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Coherent electronic transport in periodic crystals

Eric Cancès†, Clotilde Fermanian Kammerer*, Antoine Levitt†, Sami Siraj-Dine†*

November 9, 2020

Abstract

We consider independent electrons in a periodic crystal in their ground state, and turn on a uniform electric field at some prescribed time. We rigorously define the current per unit volume and study its properties using both linear response and adiabatic theory. Our results provide a unified framework for various phenomena such as the quantization of Hall conductivity of insulators with broken time-reversibility, the ballistic regime of electrons in metals, Bloch oscillations in the long-time response of metals, and the static conductivity of graphene. We identify explicitly the regime in which each holds.

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1 Introduction

We consider a d-dimensional perfect crystal ($d = 1$, 2 or 3) with periodic lattice $\mathcal{R}$ and assume that its electronic structure can be described by an effective linear Hamiltonian H acting on some Hilbert space $\mathcal{H}$. We focus here on the case of spinless continuous models, for which $\mathcal{H} = L^2(\mathbb{R}^d;\mathbb{C})$ and

$$H = \frac{1}{2}(-i\nabla + \mathcal{A})^2 + V, \tag{1}$$

where $\mathcal{A} \in L^4_{\rm per}(\mathbb{R}^d;\mathbb{R}^d)$ and $V \in L^2_{\rm per}(\mathbb{R}^d;\mathbb{R})$ are $\mathcal{R}$-periodic functions. We adopt the Coulomb gauge choice, $\nabla\cdot\mathcal{A} = 0$ in the sense of distributions. At zero temperature, the ground-state density matrix is given by

$$\gamma(0) = \mathbb{1}(H \le \mu_{\rm F}), \tag{2}$$

where $\mu_{\rm F} \in \mathbb{R}$ is the Fermi level, chosen to have a prescribed number of electrons per unit cell.

Depending on the position of $\mu_{\rm F}$ in the spectrum $\sigma(H)$ of H, this can model different types of physical systems. If $\mu_{\rm F} \notin \sigma(H)$, the system is an insulator. If $\mu_{\rm F}$ is an interior point of $\sigma(H)$, the system is a metal, or a semi-metal, depending on the density of states of H at $\mu_{\rm F}$. We refer to Section 2.4 for the precise hypotheses we use in each case.

The vector potential $\mathcal{A}$ is chosen to be periodic, which excludes the case of a uniform external magnetic field. Our analysis therefore does not directly cover the quantum Hall effect, but can be adapted to do so (see Remark 2.3). It is directly applicable to the quantum anomalous Hall effect [20]. We perform our analysis with this particular Hamiltonian, but it can easily be extended to spin-dependent continuous models, tight-binding models, or 2D materials such as graphene (for which the physical space is three-dimensional while the periodic lattice is two-dimensional); see Remark 2.3 for the exact structure needed.

The purpose of this article is to analyze mathematically the behavior of the electrical current appearing in the crystal when a uniform external electric field is turned on instantaneously at the initial time $t = 0$. In the case of a uniform stationary electric field of magnitude $\varepsilon > 0$ along a (not necessarily normalized) vector $e_\beta \in \mathbb{R}^d$, the Hamiltonian of the system at time $t > 0$ is

$$H^\varepsilon_\beta = H + \varepsilon x_\beta, \tag{3}$$

where $x_\beta = x \cdot e_\beta$. This operator is self-adjoint on $L^2(\mathbb{R}^d;\mathbb{C})$ (see Proposition 2.2 below), and therefore gives rise to a unitary group $(\mathrm{e}^{-itH^\varepsilon_\beta})_{t\in\mathbb{R}}$ on $L^2(\mathbb{R}^d;\mathbb{C})$. The electronic state of the system at time $t \ge 0$ then is

$$\gamma^\varepsilon_\beta(t) = \mathrm{e}^{-itH^\varepsilon_\beta}\gamma(0)\mathrm{e}^{itH^\varepsilon_\beta}. \tag{4}$$

The electrical current in the e_α-direction at time $t \ge 0$ is defined as

$$j^\varepsilon_{\alpha,\beta}(t) = \underline{\mathrm{Tr}}(J_\alpha\gamma^\varepsilon_\beta(t)), \tag{5}$$

where $\underline{\mathrm{Tr}}$ is the trace per unit volume (which will be precisely defined in Section 2.1) and J_α the current operator along the vector $e_\alpha \in \mathbb{R}^d$ (not necessarily normalized nor orthogonal to e_β), defined as

$$J_\alpha = -\,(-i\nabla + \mathcal{A})\cdot e_\alpha. \tag{6}$$

Remark 1.1 (on units and sign convention). If a spinless particle with mass m and charge q is subjected to a electromagnetic field generated by a vector potential $\mathcal{A}$ and a scalar potential $-\varepsilon x_\beta$ generated by a uniform electric field εe_β, its Hamiltonian in atomic units is $H = \frac{1}{2m}(-i\nabla - q\mathcal{A})^2 - q\varepsilon x_\beta$ and the charge current operator is $J = q(-i\nabla - q\mathcal{A})$. In our definitions (1), (3) and (6), we have set $m = 1$ and $q = -1$ (atomic units) which are the physical values for the electron: this corresponds to applying a force in the direction $-e_\beta$ to the electrons, and measuring their velocity in the direction $-e_\alpha$.

In the limit of weak external fields ($\varepsilon \ll 1$), the qualitative properties of the function $t \mapsto j^\varepsilon_{\alpha,\beta}(t)$ heavily depends on the physical nature of the material (insulator, metal, semi-metal), as well as on the regime (short, intermediate or long times). Our main results, stated in Theorems 2.7, 2.8 and 2.10, show that the behavior is as follows (see Figure 2 in Section 3)

- For insulators, the time-averaged conductivity

$$\sigma_{\alpha,\beta} = \lim_{t\to\infty}\frac{1}{t}\int_0^t \lim_{\varepsilon\to 0}\frac{j^\varepsilon_{\alpha,\beta}(t')}{\varepsilon}\,dt' \tag{7}$$

  has a finite value, which is zero in longitudinal directions, and, for 2D materials, is proportional to the Chern number in the transverse direction (quantum anomalous Hall effect).

- For metals, when $t \ll \varepsilon^{-1}$, the electrons are in the ballistic regime, and the current increases linearly: $j^{\varepsilon}_{\alpha,\beta}(t) \approx D_{\alpha,\beta}\varepsilon t$. Under some additional assumptions on the Bloch bands, the current displays Bloch oscillations of order 1 when $\varepsilon^{-1} \ll t \ll \varepsilon^{-1}\log(\varepsilon^{-\zeta})$ for some small enough $\zeta > 0$.
- For time-reversible 2D semimetals such as graphene, the time-averaged conductivity $\sigma_{\alpha,\beta}$ defined in (7) has a finite value equal to $\frac{1}{16} e_\alpha \cdot e_\beta$ times the number of Dirac points in the Brillouin zone.

Although our formalism is different, our results for insulators and metals are formally consistent with those obtained using the semiclassical equations of motion $\dot{x} = \nabla\lambda_{n,k},\ \dot{k} = -\nabla V + \dot{x} \times (\nabla \times \mathcal{A})$ and their higher-order refinements in the case when the n^{th} band is isolated, where the $\lambda_{n,k}$'s are the Bloch eigenvalues of H (see Section 2.1). We refer to [30, 35] for a mathematical analysis of the insulating case.

Note that our results use an averaging in time, and we are unable to conclude anything about what would be the naive definition of the conductivity

$$\lim_{t\to\infty} \lim_{\varepsilon\to 0} \frac{j^{\varepsilon}_{\alpha,\beta}(t)}{\varepsilon}. \tag{8}$$

A form of averaging of time fluctuations is always necessary to infer zero-frequency behavior from step responses in non-dissipative systems, even in the linear case. The easiest way to see this is by the very simple model for the relationship between an input $I(t)$ and an output $O(t)$:

$$i\dot{O}(t) = \omega O(t) + I(t). \tag{9}$$

This simplified model describes a forced oscillator with eigenfrequency ω, and arises from the linear response of the time-dependent Schrödinger equation of a two-level system. For a constant input I_0, there is a steady state solution $O_0 = \widehat{R}_0 I_0$, where $\widehat{R}_0 = -\frac{1}{\omega}$ is the zero-frequency transfer function of the system. However, since this system is oscillatory, this steady state may never be reached: if I is brutally switched on at time 0 with $I(t) = O(t) = 0$, if $t \le 0$, $I(t) = I_0$ if $t > 0$, then $O(t) = O_0(1 - \mathrm{e}^{-i\omega t}) = \widehat{R}_0 I_0 (1 - \mathrm{e}^{-i\omega t})$ and we cannot define $\widehat{R}_0$ as the limit of $O(t)/I_0$ when t goes to infinity. However, by averaging we obtain

$$\lim_{t\to\infty} \frac{1}{t} \int_0^t \frac{O(t')}{I_0}\, dt' = \widehat{R}_0.$$

Another common way of retrieving the value of $\widehat{R}_0$ is by an adiabatic switching of the electric field $I(t) = I_0 \mathrm{e}^{\eta t}$ for $t \le 0$, $I(t) = I_0$ for $t > 0$ [5, 9]. Another possibility is to represent the relationship between O and I by a convolution with a causal response function $R(t)$: $O(t) = (R * I)(t)$, and define the zero-frequency transfer function as $\lim_{\eta\to 0^+} \widehat{R}(i\eta)$, as is often done implicitly in the physics literature. Yet another, more physical, possibility is to use a model with dissipation (in this case $i\dot{O}_\eta(t) + i\eta O_\eta(t) = \omega O_\eta(t) + I(t)$), compute the zero-frequency transfer function as the long-time limit of $O_\eta(t)/I_0$, and then let the dissipation η tend to zero. A particular variant of this scheme is known as the relaxation time approximation [3] (the relaxation time being proportional to $1/\eta$). For simple systems, all these methods are equivalent.

Note that the problems in the toy model (9) are related to the presence of a *resonance* at ω in the model, i.e. a pole in the Fourier transform of the response function. For our perfect crystal model however, the oscillatory components of the response are integrated over the Brillouin zone of the periodic crystal, which induces an averaging. Therefore, these procedures might not be necessary. Indeed, we observe numerically in simple tight-binding models that the naive limit in (8) seems to be well-defined (see Section 3). Identifying precise conditions on the band structure so that this holds will be the subject of future work.

In the metallic case, the conductivity is either infinity or zero, depending on the definition adopted. Indeed, our results imply that

$$\lim_{t\to\infty} \frac{1}{t} \int_0^t \lim_{\varepsilon\to 0} \frac{j^{\varepsilon}_{\alpha,\alpha}(t')}{\varepsilon}\, dt' = +\infty$$

is infinite, because $j^{\varepsilon}_{\alpha,\alpha}(t) \approx D_{\alpha\alpha}\varepsilon t$ in the regime $t \ll \varepsilon^{-1}$. On the other hand, in tight-binding models, a simple argument [3, Proposition 4] shows that

$$\lim_{\varepsilon\to 0} \frac{1}{\varepsilon} \lim_{t\to\infty} \frac{1}{t} \int_0^t j^{\varepsilon}_{\alpha,\alpha}(t')\, dt' = 0.$$

These two limits correspond to different regimes. In the first one, the electrons undergo ballistic transport, being uniformly accelerated by the electric field. In the second one, the electrons undergo Bloch oscillations, a phenomenon whereby particles in a periodic potential accelerated by a constant force oscillate rather than propagate, as first noticed by Zener [43].

Of course, our model is extremely simple. We assume that the electrons are at zero temperature and we ignore electron-electron interactions, the reaction of the lattice (electron-phonon interactions), and electron scattering by impurities in the crystal. These collision events play a relatively minor role in insulators at low temperatures, with the quantum Hall effect in particular being very robust to perturbations [3]. However, they impact significantly the properties of metals. In fact, in the linear response regime ($\varepsilon \ll 1$, $t \ll \varepsilon^{-1}$), the current increases linearly, representing ballistic transport (see Theorem 2.8). This increase in the velocity of the electrons physically results in an increased collision rate, which acts as dissipation and eventually limits the current. This results in the finite conductivity observed experimentally in macroscopic physics (Ohm's law). The mathematical understanding of this effect in the mathematical framework considered here is left to future work.

The question of quantum transport in solids has attracted significant attention in the mathematical community, with one of the main drivers being the explanation of Anderson localization on the one hand, and the quantum Hall effect and its relation to topological properties on the other hand [37, 28, 15, 29, 26]. Other topics of interest include the properties of graphene (see for instance [18]), and mesoscopic transport in the Landauer-Buttiker formalism. Comparatively few works have looked specifically at transport in metals. To the best of our knowledge, the present work is the first to present mathematically rigorous results on insulators, metals and semi-metals in a unified framework.

In our results in the linear response regime, we consider the quantity

$$j^{\mathrm{LR}}_{\alpha,\beta}(t) = \lim_{\varepsilon\to 0} \frac{j^{\varepsilon}_{\alpha,\beta}(t)}{\varepsilon}.$$

and then compute the conductivity in the limit $t \to \infty$. This order of limits is necessary to ensure that the electronic state never deviates significantly from its equilibrium. Considering the opposite limit, i.e. the infinite-time dynamics of $j^{\varepsilon}_{\alpha,\beta}(t)$ at ε fixed, is an extremely hard problem, as it is for any dynamics of non-dissipative systems.

The validity of this linear response approximation to derive conductivities, pioneered by Kubo in [22], is by no means obvious. As was pointed out in [39], the most obvious way to derive it, "microscopic linearity" is not physically relevant: assuming a mean free path length d for the electrons, the validity condition that a free electron of (effective) mass m and charge e is not significantly affected by an electric field E in the time interval $[0, t]$ is $\frac{t^2}{2}\frac{eE}{m} \ll d$. Taking macroscopic times t and reasonable microscopic values for e and m, this limits fields to microscopic values ([39] quotes 10^{-18} Volt/cm), which is unrealistic in practice. The solution of this paradox is "macroscopic linearity": $\gamma^{\varepsilon}_{\beta}(t)$ has to be understood not as the state of a single set of electrons, but rather as a thermodynamic ensemble. The effective evolution of $\gamma^{\varepsilon}_{\beta}(t)$ then involves a dissipative term (coming from electron-phonon, electron-impurity or electron-electron interaction) that tends to restore the density matrix to its equilibrium state. The condition of validity of linear response is then that the driving force is negligible compared to the restoring force, which is usually satisfied in practice [40]. The mathematical justification of linear response is then to consider a more sophisticated model involving a dissipation strength η, and to perform the van Hove limit $t \to \infty, \eta \to 0, t^2\eta = \mathrm{cst}$, at ε fixed [40]. Then ε can be taken to zero, and the results of linear response are recovered. Alternatively, a Drude-type model like the relaxation-time approximation [2] can be used, with the similar effect of returning the density matrix to equilibrium. Yet another possibility is to never let the density matrix get out of its equilibrium state by switching on adiabatically the external field from negative infinity as $e^{\eta t}\varepsilon x_\beta$, and to consider the limit $\eta \to 0$ first then $\varepsilon \to 0$ [1]. In our naive model, we do not consider a dissipation term, and therefore simply assume the validity of linear response.

Our method of proof is based on the standard gauge change $\widetilde{\psi}(x, t) = \mathrm{e}^{i\varepsilon t x_\beta}\psi(x, t)$ that transforms the constant in time but non-spatially-periodic Hamiltonian $H^{\varepsilon}_{\beta} = H + \varepsilon x_\beta$ into the time-dependent Hamiltonian $\widetilde{H}^{\varepsilon}_{\beta}(t) = \frac{1}{2}(-i\nabla + \mathcal{A} - \varepsilon e_\beta t)^2 + V$. This Hamiltonian is spatially periodic, and the study of its dynamics can be reduced via Bloch-Floquet theory to that of its fibers $\widetilde{H}^{\varepsilon}_{\beta,k}(t) = \frac{1}{2}(-i\nabla + k + \mathcal{A} - \varepsilon e_\beta t)^2 + V$ acting on periodic functions (Section 4), for all values of the pseudo-momentum $k \in \mathbb{R}^d$. Fiber by fiber, this time-dependent Hamiltonian can then be treated using the tools of time-dependent perturbation theory (Section 5). Since time is scaled by ε, the Hamiltonian can be seen as either a small perturbation of the rest Hamiltonian H for small times (in which case we can use linear response to expand $j^{\varepsilon}_{\alpha,\beta}(t)$ to first order in ε for a fixed t, Proposition 5.7), or as a slow perturbation (in which case the adiabatic theorem allows us to access larger time scales $t \approx \frac{1}{\varepsilon}$, Proposition 5.3). For insulators and metals in the short-time regime, both tools are applicable and yield the same result. For metals in the Bloch oscillations regime, only the adiabatic theorem is applicable, and for semimetals, only linear response is applicable due to the gap closing at the Dirac points.

The techniques we use (linear response and adiabatic theory) are not new, nor are our results particularly surprising to experts in the field. Rather, we see the contribution of this paper as unifying in the same framework disparate studies on different systems, as well as providing insights on the current response without any specific regularization technique (such as adiabatic switching or dissipation). Our results on Bloch oscillations also appear to be new in the mathematical literature.

The structure of the paper is as follows. We describe our results in Section 2: we define the current in Proposition 2.2, and study its properties for insulators, metals and semi-metals in Theorems 2.7, 2.8 and 2.10. We illustrate numerically the different behaviors we obtain in each of the three settings in Section 3. We devote Section 4 to preliminaries about the regularity and Bloch decomposition of the current. Section 5 states and proves results in adiabatic and linear response perturbation theory. Sections 6, 7 and 8 are devoted to the proof of our results in the case of insulators, metals and semi-metals. Finally two short Appendices are devoted to technical issues.

2 Main results: electrical current in periodic materials

2.1 Notation

In this paper we fix $\mathcal{A} \in L^4_{\rm per}(\mathbb{R}^d;\mathbb{R}^d)$, $V \in L^2_{\rm per}(\mathbb{R}^d;\mathbb{R})$ (see below for the definition of these spaces), $\mu_{\rm F} \in \mathbb{R}$, and $\mathcal{R}$ is the lattice of the d-dimensional crystal. We fix a (non-necessarily orthonormal) basis $(e_\alpha)_{\alpha=1,\dots,d}$ of the momentum space $\mathbb{R}^d$, and set $x_\alpha = x \cdot e_\alpha, \mathcal{A}_\alpha = \mathcal{A} \cdot e_\alpha$ for $\alpha = 1,\dots,d$. We denote by $\mathcal{R}^*$ the *dual lattice* of the periodic lattice $\mathcal{R}$, by Ω an arbitrary unit cell in the physical space, and by $\mathcal{B}$ an arbitrary unit cell in the reciprocal space (which we will call by abuse of language the *Brillouin zone*). In the special case of a cubic crystal of lattice parameter $a > 0$, we have $\mathcal{R} = a\mathbb{Z}^d$, $\mathcal{R}^* = \frac{2\pi}{a}\mathbb{Z}^d$, and we can take $\Omega = [0,a)^d$, $\mathcal{B} = [-\frac{\pi}{a},\frac{\pi}{a})^d$.

The *$\mathcal{R}$-periodic Lebesgue and Sobolev spaces* are denoted by

$$L^p_{\rm per} := \left\{u \in L^p_{\rm loc}(\mathbb{R}^d;\mathbb{C}) \mid u \ \mathcal{R}\text{-periodic}\right\},$$
$$H^s_{\rm per} := \left\{u \in H^s_{\rm loc}(\mathbb{R}^d;\mathbb{C}) \mid u \ \mathcal{R}\text{-periodic}\right\}.$$

The space of bounded linear operators on a Hilbert space $\mathcal{H}$ is denoted by $\mathcal{L}(\mathcal{H})$, and the Schatten class of bounded operators $A \in \mathcal{L}(\mathcal{H})$ such that $\mathrm{Tr}(|A|^p) < \infty$ by $\mathfrak{S}_p(\mathcal{H})$. For $R \in \mathcal{R}$, we denote by τ_R the translation operator formally defined by $\tau_R\phi = \phi(\cdot - R)$. Depending on the context, τ_R will be seen as a unitary operator on $L^2(\mathbb{R}^d;\mathbb{C})$, or as a linear operator on some $\mathcal{R}$-translation invariant subspace of $\mathcal{D}'(\mathbb{R}^d;\mathbb{C})$. A bounded operator on $L^2(\mathbb{R}^d;\mathbb{C})$ is called $\mathcal{R}$-periodic if it commutes with τ_R for all $R \in \mathcal{R}$. An unbounded self-adjoint operator on $L^2(\mathbb{R}^d;\mathbb{C})$ is called $\mathcal{R}$-periodic if its resolvent is $\mathcal{R}$-periodic. A bounded $\mathcal{R}$-periodic operator $A \in \mathcal{L}(L^2(\mathbb{R}^d;\mathbb{C}))$ is called locally trace-class if $\chi A \chi \in \mathfrak{S}_1(L^2(\mathbb{R}^d;\mathbb{C}))$ for any compactly supported function $\chi \in L^\infty(\mathbb{R}^d;\mathbb{C})$. For $p \geq 1$, we denote by $\mathfrak{S}_{p,\rm per}$ the space of $\mathcal{R}$-periodic operators $A \in \mathcal{L}(L^2(\mathbb{R}^d;\mathbb{C}))$ such that $|A|^p$ is locally trace class. Any operator $A \in \mathfrak{S}_{1,\rm per}$ has a density $\rho_A \in L^1_{\rm per}$ characterized by

$$\forall \chi \in C^\infty_{\rm c}(\mathbb{R}^d;\mathbb{C}), \quad \mathrm{Tr}(A\chi) = \int_{\mathbb{R}^d} \rho_A \chi.$$

The trace per unit volume of an operator $A \in \mathfrak{S}_{1,\rm per}$ is defined as

$$\underline{\mathrm{Tr}}(A) = \frac{1}{|\Omega|}\mathrm{Tr}_{L^2(\mathbb{R}^d;\mathbb{C})}(\mathbb{1}_\Omega A \mathbb{1}_\Omega) = \fint_\Omega \rho_A,$$

where $\mathbb{1}_\Omega$ is the characteristic function of the unit cell Ω, and $\fint_\Omega$ is a shorthand notation for $\frac{1}{|\Omega|}\int_\Omega$. This formula is independent of the choice of the unit cell Ω.

Since we are dealing here with periodic materials, we will use the Bloch transform (also called Bloch-Floquet transform) [33, 23, 41]. For $K \in \mathcal{R}^*$, let T_K be the unitary multiplication operator on $L^2_{\rm per}$ defined by

$$\forall v \in L^2_{\rm per}, \quad (T_K v)(x) = \mathrm{e}^{-iK\cdot x} v(x) \quad \text{ for a.a. } x \in \mathbb{R}^d,$$

and

$$L^2_{\rm qp}(L^2_{\rm per}) \\ := \left\{ \mathbb{R}^d \ni k \mapsto u_k \in L^2_{\rm per} \mid \int_{\mathcal{B}} \|u_k\|^2_{L^2_{\rm per}} \, dk < \infty, \ u_{k+K} = T_K u_k \text{ for all } K \in \mathcal{R}^* \text{ and a.a. } k \in \mathbb{R}^d \right\},$$

the Hilbert space of $\mathcal{R}^*$-quasi-periodic $L^2_{\rm per}$-valued functions on $\mathbb{R}^d$ endowed with the inner product

$$\langle u, v \rangle_{L^2_{\rm qp}(L^2_{\rm per})} = \fint_{\mathcal{B}} \langle u_k, v_k \rangle_{L^2_{\rm per}} \, dk.$$

Here and below, the subscript qp refers to the quasi-periodicity property. The Bloch transform then is the unitary map from $L^2(\mathbb{R}^d; \mathbb{C})$ to $L^2_{\rm qp}(L^2_{\rm per})$ defined for $u \in C^\infty_{\rm c}(\mathbb{R}^d; \mathbb{C})$ by

$$\forall k \in \mathbb{R}^d, \quad \forall x \in \mathbb{R}^d, \quad u_k(x) = \sum_{R \in \mathcal{R}} u(x+R) \, \mathrm{e}^{-ik\cdot(x+R)}. \tag{10}$$

Its inverse is given by

$$u(x) = \fint_{\mathcal{B}} \mathrm{e}^{ik\cdot x} u_k(x) \, dk, \quad \text{ for a.a. } x \in \mathbb{R}^d. \tag{11}$$

Any $\mathcal{R}$-periodic operator $A \in \mathcal{L}(L^2(\mathbb{R}^d; \mathbb{C}))$ is decomposed by the Bloch transform in the sense that there exists a function $k \mapsto A_k$ in $L^\infty_{\rm qp}(\mathcal{L}(L^2_{\rm per}))$ such that for any $u \in L^2(\mathbb{R}^d; \mathbb{C})$ and almost all $k \in \mathbb{R}^d$, $(Au)_k = A_k u_k$, and

$$A_{k+K} = T_K A_k T_K^*, \quad \text{ for all } K \in \mathcal{R}^* \text{ and a.a. } k \in \mathbb{R}^d. \tag{12}$$

The A_k's are called the fibers of the operator A. If $A \in \mathfrak{S}_{1,\rm per}$, then the function $k \mapsto A_k$ is in $L^1_{\rm qp}(\mathfrak{S}_1(L^2_{\rm per}))$, the function $k \mapsto \mathrm{Tr}(A_k)$ is in $L^1_{\rm loc}(\mathbb{R}^d)$, $\mathcal{R}^*$-periodic, and we have

$$\underline{\mathrm{Tr}}(A) = (2\pi)^{-d} \int_{\mathcal{B}} \mathrm{Tr}(A_k) \, dk.$$

The Bloch decomposition theorem can be extended to unbounded $\mathcal{R}$-periodic self-adjoint operators using the resolvent [33].

In the case of the periodic Hamiltonian operator H given by (1), we have

$$H_k = \frac{1}{2}(-i\nabla + k + \mathcal{A})^2 + V. \tag{13}$$

For each $k \in \mathbb{R}^d$, H_k is a bounded below self-adjoint operator on $L^2_{\rm per}$ with domain $H^2_{\rm per}$ and compact resolvent. Let $(\lambda_{n,k})_{n\in\mathbb{N}^*}$ be the non-decreasing sequence of eigenvalues of H_k counting multiplicities

$$\lambda_{1,k} \le \lambda_{2,k} \le \lambda_{3,k} \le \cdots, \quad \lim_{n\to\infty} \lambda_{n,k} = +\infty,$$

and we use the convention $\lambda_{0,k} = -\infty$. We denote by $(u_{n,k})_{n\in\mathbb{N}^*} \in (H^2_{\rm per})^{\mathbb{N}^*}$ an $L^2_{\rm per}$-orthonormal basis of associated eigenfunctions:

$$H_k u_{n,k} = \lambda_{n,k} u_{n,k}, \quad \langle u_{m,k}, u_{n,k} \rangle_{L^2_{\rm per}} = \delta_{m,n}.$$

For $N \in \mathbb{N}^*$ and $k \in \mathbb{R}^d$, we will denote by

$$P_{N,k} = \mathbb{1}(H_k \le \lambda_{N,k}). \tag{14}$$

Whenever $\lambda_{N,k} < \lambda_{N+1,k}$, $P_{N,k}$ is the spectral projector on the eigenspace associated with the lowest N eigenvalues of H_k (counting multiplicities):

$$P_{N,k} = \sum_{n=1}^{N} |u_{n,k}\rangle\langle u_{n,k}|. \tag{15}$$

Since H_k is quasi-periodic, so is $P_{N,k}$, and the eigenvalues $\lambda_{n,k}$ are $\mathcal{R}^*$-periodic functions of k. By a min-max argument (see e.g. [33, 6]), there exists $\underline{C_1}, \overline{C_1} \in \mathbb{R}$, and $\underline{C_2}, \overline{C_2} > 0$ such that

$$\underline{C_1} + \underline{C_2} n^{2/d} \leq \lambda_{n,k} \leq \overline{C_1} + \overline{C_2} n^{2/d}. \tag{16}$$

Denoting by N_k the number of eigenvalues below the Fermi level μ_{F} at k

$$N_k = \left| \left\{ \lambda_{n,k} \leq \mu_{\mathrm{F}}, n \in \mathbb{N}^* \right\} \right|, \tag{17}$$

we see that N_k is bounded uniformly in k.

Let us now consider the ground-state density matrix $\gamma(0) = \mathbb{1}(H \leq \mu_{\mathrm{F}})$ defined in (2). Its Bloch fibers are

$$\gamma_k(0) = \mathbb{1}(H_k \leq \mu_{\mathrm{F}}) = P_{N_k,k}. \tag{18}$$

The *current operator* $J_\alpha = -(-i\nabla + \mathcal{A}) \cdot e_\alpha$ defined in (6) is also $\mathcal{R}$-periodic, with fibers

$$J_{\alpha,k} = -(-i\nabla + k + \mathcal{A}) \cdot e_\alpha = -\nabla_k H_k \cdot e_\alpha =: -\partial_\alpha H_k.$$

Note that the notation ∂_α denotes a derivative along the (not necessarily normalized) vector e_α.

Lastly, for each $q \in \mathbb{R}^d$, we denote that G_q the unitary multiplication operator on $L^2(\mathbb{R}^d; \mathbb{C})$ defined by

$$\forall u \in L^2(\mathbb{R}^d; \mathbb{C}), \quad (G_q u)(x) = \mathrm{e}^{iq\cdot x} u(x) \quad \text{ for a.a. } x \in \mathbb{R}^d. \tag{19}$$

The operator G_q is not $\mathcal{R}$-periodic, except when $q \in \mathcal{R}^*$ (in which case G_q is fibered, with $G_{q,k} = T_{-q}$ for all k). However, for any $\mathcal{R}$-periodic operator $A \in \mathcal{L}(L^2(\mathbb{R}^d; \mathbb{C}))$ and any $q \in \mathbb{R}^d$, the operator $G_q A G_q^*$ is $\mathcal{R}$-periodic and its Bloch decomposition is given by

$$(G_q A G_q^*)_k = A_{k-q}, \quad \text{ for a.a. } k \in \mathbb{R}^d. \tag{20}$$

2.2 The Bloch theorem

Before attacking the well-posedness of the current $j^\varepsilon_{\alpha,\beta}(t) = \underline{\mathrm{Tr}}(J_\alpha \gamma^\varepsilon_\beta(t))$ for $\varepsilon, t \neq 0$, we first study an easier special case.

Proposition 2.1 (Bloch theorem)**.** *The current satisfies*

$$\begin{aligned}
j^0_{\alpha,\beta}(t) &= 0, \quad \forall t \geq 0 \quad \textit{(no current in the absence of external field)},\\
j^\varepsilon_{\alpha,\beta}(0) &= 0, \quad \forall \varepsilon \geq 0 \quad \textit{(continuity of the current at } t = 0\textit{)}.
\end{aligned}$$

Proof. This is a classical statement going back to Bloch, valid in a more general context. We adapt here the proof in [4]. We have

$$J := j^0_{\alpha,\beta}(t) = j^\varepsilon_{\alpha,\beta}(0) = \underline{\mathrm{Tr}}(J_\alpha \gamma(0)) = -(2\pi)^{-d} \int_{\mathcal{B}} \mathrm{Tr}(\partial_\alpha H_k \gamma_k(0))\, dk.$$

Assume that this quantity is non-zero. Construct for $\delta \in \mathbb{R}$ a trial state

$$\gamma^\delta = e^{-i\delta e_\alpha x} \gamma(0) e^{i\delta e_\alpha x},$$

a periodic operator with fibers

$$\gamma^\delta_k = \gamma_{k+\delta e_\alpha},$$

and compute

$$\begin{aligned}
\underline{\mathrm{Tr}}(H\gamma^\delta) &= (2\pi)^{-d} \int_{\mathcal{B}} \mathrm{Tr}(H_k \gamma_{k+\delta e_\alpha}(0))\, dk\\
&= (2\pi)^{-d} \int_{\mathcal{B}} \mathrm{Tr}(H_{k-\delta e_\alpha} \gamma_k(0))\, dk\\
&= \underline{\mathrm{Tr}}(H\gamma(0)) - \delta (2\pi)^{-d} \int_{\mathcal{B}} \mathrm{Tr}(\partial_\alpha H_k \gamma_k(0))\, dk + O(\delta^2).
\end{aligned}$$

Since $\gamma(0)$ is the ground state, $\underline{\mathrm{Tr}}(H\gamma^\delta) \leq \underline{\mathrm{Tr}}(H\gamma(0))$ for all δ, and therefore $J = 0$.

□

2.3 Definition of the current

For $\varepsilon > 0$, the operator

$$H_\beta^\varepsilon = H + \varepsilon x_\beta = \frac{1}{2}(-i\nabla + \mathcal{A})^2 + V + \varepsilon x \cdot e_\beta$$

already introduced in (3) is not $\mathcal{R}$-periodic, and we would naively expect that the density matrix

$$\gamma_\beta^\varepsilon(t) = \mathrm{e}^{-itH_\beta^\varepsilon}\gamma(0)\mathrm{e}^{itH_\beta^\varepsilon}$$

at time $t > 0$ (already introduced in (4)) is not either. Yet, this operator is in fact $\mathcal{R}$-periodic. Physically, this is due to the fact that although the potential $V_{\mathrm{el}}(x) := \varepsilon x \cdot e_\beta$ is not periodic, the field $\mathcal{E} = -\nabla V_{\mathrm{el}} = -\varepsilon e_\beta$ to which the electrons are subjected is constant, hence periodic. The proof of this result relies on the standard gauge transform

$$\widetilde{\psi}(x,t) = \left((G_{\varepsilon t e_\beta}\psi(\cdot,t)\right)(x) = \mathrm{e}^{i\varepsilon t x_\beta}\psi(x,t), \tag{21}$$

where the operator G_q has been defined in (19), and the introduction of the gauge-transformed operators

$$\widetilde{\mathcal{U}}_\beta^\varepsilon(t,t') := G_{\varepsilon t e_\beta}\mathrm{e}^{-i(t-t')H_\beta^\varepsilon}G_{\varepsilon t' e_\beta}^*, \tag{22}$$

and

$$\widetilde{\gamma}_\beta^\varepsilon(t) := G_{\varepsilon t e_\beta}\gamma_\beta^\varepsilon(t)G_{\varepsilon t e_\beta}^* = \widetilde{\mathcal{U}}_\beta^\varepsilon(t)\gamma(0)\widetilde{\mathcal{U}}_\beta^\varepsilon(t)^*, \tag{23}$$

where $\widetilde{\mathcal{U}}_\beta^\varepsilon(t)$ is a short-hand notation for

$$\widetilde{\mathcal{U}}_\beta^\varepsilon(t) := \widetilde{\mathcal{U}}_\beta^\varepsilon(t,0) = G_{\varepsilon t e_\beta}\mathrm{e}^{-itH_\beta^\varepsilon}.$$

Through the change of gauge (21), the dynamics induced by the time-independent but non-periodic Hamiltonian H_β^ε is equivalent to the dynamics induced by the time-dependent periodic Hamiltonian

$$\widetilde{H}_\beta^\varepsilon(t) = G_{\varepsilon t e_\beta}H_\beta^\varepsilon G_{\varepsilon t e_\beta}^* = \frac{1}{2}(-i\nabla + \mathcal{A} - \varepsilon e_\beta t)^2 + V. \tag{24}$$

This change of gauge is standard in both the mathematical and physical literature, as it turns the spatially inhomogeneous electric potential $V_{\mathrm{el}} = -\varepsilon x_\beta$ into a homogeneous (but time-dependent) magnetic potential $\mathcal{A}_{\mathrm{el}} = -\varepsilon e_\beta t$, more convenient to deal with here because it does not break periodicity. Physically, this is a manifestation of the gauge invariance of the Schrödinger equation, where an electric field $\mathcal{E} = -\nabla V_{\mathrm{el}} - \frac{\partial \mathcal{A}_{\mathrm{el}}}{\partial t}$ can be realized either through a scalar or vector potential. The Bloch fibers of $\widetilde{H}_\beta^\varepsilon(t)$ are

$$\widetilde{H}_{\beta,k}^\varepsilon(t) = \frac{1}{2}(-i\nabla + k + \mathcal{A} - \varepsilon e_\beta t)^2 + V = H_{k-\varepsilon e_\beta t}. \tag{25}$$

We sum up these arguments in the proposition below, together with elements that we shall use for defining the current. The reader can refer to the articles [5, 24] where part of the results of that Proposition are proved.

Proposition 2.2. *Let $\mathcal{A} \in L^4_{\mathrm{per}}(\mathbb{R}^d;\mathbb{R}^d)$ such that $\nabla \cdot \mathcal{A} = 0$, and $V \in L^2_{\mathrm{per}}(\mathbb{R}^d;\mathbb{R})$.*

1. *For all $\varepsilon \in \mathbb{R}$, the operator H_β^ε defined in (3) is essentially self-adjoint on $C_c^\infty(\mathbb{R}^d;\mathbb{C})$, and therefore admits a unitary propagator $(\mathrm{e}^{-itH_\varepsilon^\beta})_{t\in\mathbb{R}}$ in $L^2(\mathbb{R}^d;\mathbb{C})$.*
2. *For all $t \in \mathbb{R}$, and $\varepsilon \in \mathbb{R}$, the operator $\widetilde{H}_\beta^\varepsilon(t)$ defined in (24) is self-adjoint on $L^2(\mathbb{R}^d)$ with domain $H^2(\mathbb{R}^d;\mathbb{C})$, and $\mathcal{R}$-periodic. The strongly continuous unitary propagator $(\widetilde{\mathcal{U}}_\beta^\varepsilon(t,t'))_{(t,t')\in\mathbb{R}\times\mathbb{R}}$ on $L^2(\mathbb{R}^d;\mathbb{C})$ defined in (22) is $\mathcal{R}$-periodic for all $t,t' \in \mathbb{R}$, with fibers $\widetilde{\mathcal{U}}_{\beta,k}^\varepsilon(t,t')$ solving*

$$i\partial_t\widetilde{\mathcal{U}}_{\beta,k}^\varepsilon(t,t') = \widetilde{H}_{\beta,k}^\varepsilon(t)\widetilde{\mathcal{U}}_{\beta,k}^\varepsilon(t,t'), \quad \widetilde{\mathcal{U}}_{\beta,k}^\varepsilon(t',t') = \mathrm{Id}_{L^2_{\mathrm{per}}}. \tag{26}$$

3. *For all $t \geq 0$, and $\varepsilon \in \mathbb{R}$, $J_\alpha\gamma_\beta^\varepsilon(t) \in \mathfrak{S}_{1,\mathrm{per}}$. The current $j_{\alpha,\beta}^\varepsilon(t) = \underline{\mathrm{Tr}}(J_\alpha\gamma_\beta^\varepsilon(t))$ is well-defined and*

$$j_{\alpha,\beta}^\varepsilon(t) = -(2\pi)^{-d}\int_{\mathcal{B}} \mathrm{Tr}\Big(\partial_\alpha\widetilde{H}_{\beta,k}^\varepsilon(t)\widetilde{\gamma}_{\beta,k}^\varepsilon(t)\Big)\,dk \tag{27}$$

$$= -(2\pi)^{-d}\int_{\mathcal{B}} \mathrm{Tr}\Big(\partial_\alpha H_{k-\varepsilon e_\beta t}\widetilde{\mathcal{U}}_{\beta,k}^\varepsilon(t)\gamma_k(0)\widetilde{\mathcal{U}}_{\beta,k}^\varepsilon(t)^*\Big)\,dk \tag{28}$$

$$
\begin{tikzcd}
\gamma(0) \arrow[r, "\mathrm{e}^{-itH^{\varepsilon}_{\beta}}"] \arrow[d, "Id"] & \gamma^{\varepsilon}_{\beta}(t) \arrow[d, "G_{\varepsilon t e_\beta}"] \\
\widetilde{\gamma}(0) \arrow[r, "\widetilde{\mathcal{U}}^{\varepsilon}_{\beta}(t)"] & \widetilde{\gamma}^{\varepsilon}_{\beta}(t)
\end{tikzcd}
$$

$$
\begin{tikzcd}
\{\gamma_k(0)\}_{k\in\mathbb{R}^d} = \{\gamma^{\varepsilon}_{\beta,k}(0)\}_{k\in\mathbb{R}^d} \arrow[r] \arrow[d, "\{Id\}_{k\in\mathbb{R}^d}"] & \{\gamma^{\varepsilon}_{\beta,k}(t)\}_{k\in\mathbb{R}^d} \arrow[d, "\text{translation in } k \text{ space by} -\varepsilon t e_\beta"] \\
\{\widetilde{\gamma}^{\varepsilon}_{\beta,k}(0)\}_{k\in\mathbb{R}^d} = \{\gamma^{\varepsilon}_{\beta,k}(0)\}_{k\in\mathbb{R}^d} \arrow[r, "\{\widetilde{\mathcal{U}}^{\varepsilon}_{\beta,k}(t)\}_{k\in\mathbb{R}^d}"] & \{\widetilde{\gamma}^{\varepsilon}_{\beta,k}(t)\}_{k\in\mathbb{R}^d} = \{\gamma^{\varepsilon}_{\beta,k-\varepsilon t e_\beta}(t)\}_{k\in\mathbb{R}^d}
\end{tikzcd}
$$

Figure 1: Commutative diagrams of the relationships between density matrices $\gamma^{\varepsilon}_{\beta}$ and $\widetilde{\gamma}^{\varepsilon}_{\beta}$ (top) and the fibers $\gamma^{\varepsilon}_{\beta,k}$ of $\gamma^{\varepsilon}_{\beta}$ which decompose both $\gamma^{\varepsilon}_{\beta}$ and $\widetilde{\gamma}^{\varepsilon}_{\beta}$ (bottom). In the top diagram, $A \xrightarrow{U} B$ means that $B = UAU^*$. In the bottom diagram $\{A_k\}_{k\in\mathbb{R}^d} \xrightarrow{\{U_k\}_{k\in\mathbb{R}^d}} \{B_k\}_{k\in\mathbb{R}^d}$ means that A and B are $\mathcal{R}$-periodic and that their fibers are related by $B_k = U_k A_k U_k^*$.

The results of Proposition 2.2 are not new (some are classical) but are nevertheless proved in Section 4 for the sake of completeness. The situation can be summed up in the commutative diagrams of Figure 1.

Remark 2.3. This proposition reduces the study of $j^{\varepsilon}_{\alpha,\beta}(t)$ to that of the dynamics of the time-dependent Hamiltonian $H_{k-\varepsilon e_\beta t}$. In particular, although we have focused on the specific Hamiltonian H given by (1), all computations beyond the proof of this proposition will be based on the use of the three formulae: for all $k \in \mathbb{R}^d, t \in \mathbb{R}_+$,

$$
\boxed{
\begin{aligned}
&\gamma_k(0) = \mathbb{1}(H_k \le \mu_{\mathrm{F}}), && (29)\\
&i\partial_t \widetilde{\mathcal{U}}^{\varepsilon}_{\beta,k}(t) = H_{k-\varepsilon e_\beta t}\widetilde{\mathcal{U}}^{\varepsilon}_{\beta,k}(t), \quad \widetilde{\mathcal{U}}^{\varepsilon}_{\beta,k}(0) = \mathrm{Id}_{\mathcal{H}_{\mathrm{f}}}, && (30)\\
&j^{\varepsilon}_{\alpha,\beta}(t) = -(2\pi)^{-d}\int_{\mathcal{B}} \mathrm{Tr}\Big(\partial_\alpha H_{k-\varepsilon e_\beta t}\widetilde{\mathcal{U}}^{\varepsilon}_{\beta,k}(t)\gamma_k(0)\widetilde{\mathcal{U}}^{\varepsilon}_{\beta,k}(t)^*\Big)\, dk, && (31)
\end{aligned}
}
$$

where the fiber $\mathcal{H}_{\mathrm{f}}$ is equal to L^2_{per} in our setting. Our results in the following sections can therefore be extended to other Hamiltonians where $(H_k)_{k\in\mathbb{R}^d}$ is a family of bounded below self-adjoint operators on a Hilbert space $\mathcal{H}_{\mathrm{f}}$ with compact resolvent satisfying the quasi-periodicity conditions

$$
H_{k+K} = T_K H_k T_K^*, \quad \forall K \in \mathcal{R}^*,\ k \in \mathbb{R}^d,
$$

where $(T_K)_{K\in\mathcal{R}^*}$ is a unitary representation of the group $\mathcal{R}^*$ on $\mathcal{H}_{\mathrm{f}}$ (see (12)), and the boundedness conditions in Section 5. This includes in particular spin-dependent continuous models, tight-binding lattice models (for which $\mathcal{H}_{\mathrm{f}} = \mathbb{C}^M$), and 2D materials. It also contains the case of systems with a constant magnetic field where the flux per unit cell satisfies an adequate commensurability condition (see [16] or [27], where ideas from [42] are implemented).

2.4 Insulators, non-degenerate metals, semimetals

As we said before, the position of the Fermi level in the band diagram $(\lambda_{n,k})_{n\in\mathbb{N}^*,\,k\in\mathcal{B}}$ is key to determining the electronic properties of the medium. We define the Fermi surface sheets

$$
\mathcal{S}_n = \{k \in \mathcal{B} \mid \lambda_{n,k} = \mu_{\mathrm{F}}\}, \quad n \in \mathbb{N}^*
$$

and the Fermi surface

$$
\mathcal{S} = \bigcup_{n\in\mathbb{N}^*} \mathcal{S}_n = \{k \in \mathcal{B} \mid \exists n \in \mathbb{N}^* \text{ s.t. } \lambda_{n,k} = \mu_{\mathrm{F}}\}. \tag{32}
$$

We will be interested here in three types of systems that we now describe in three mutually exclusive assumptions.

Assumption 2.4 (insulator)**.** *The Fermi surface $\mathcal{S}$ is empty, and there exists $N_{\text{ins}} \in \mathbb{N}^*$ such that $N_k = N_{\text{ins}}$ for all $k \in \mathcal{B}$, i.e.*

$$\forall k \in \mathcal{B}, \quad \lambda_{N_{\text{ins}},k} < \mu_{\text{F}} < \lambda_{N_{\text{ins}}+1,k},$$

or equivalently $\mu_{\text{F}} \notin \sigma(H)$.

In the case of insulators, we have for all $k \in \mathbb{R}^d$

$$\gamma_k(0) = P_{N_{\text{ins}},k},$$

and $\gamma_k(0)$ is a real-analytic $\mathcal{R}^*$-quasi-periodic function.

Assumption 2.5 (non-degenerate metal)**.** *The Fermi surface $\mathcal{S}$ is non-empty and the following conditions are satisfied: for all $n \in \mathbb{N}^*$,*

- *$\mathcal{S}_n \cap \mathcal{S}_{n+1} = \emptyset$ (no crossing at the Fermi level);*
- *for all $k \in \mathcal{S}_n$, $\nabla\lambda_{n,k} \neq 0$ (no flat bands at the Fermi level).*

Note that this assumption was used in [6]. It ensures a smooth density of states at the Fermi level. In this case, the Fermi surface consists of a finite union of disjoint smooth closed surfaces $\mathcal{S}_n$. Letting

$$\mathcal{B}_n = \{k \in \mathcal{B} \mid \lambda_{n,k} < \mu_{\text{F}} < \lambda_{n+1,k}\},$$

we obtain a partitioning

$$\mathcal{B} = \mathcal{S} \bigcup \left(\bigcup_{n\in\mathbb{N}^*} \mathcal{B}_n \right).$$

Both N_k and the fibers $\gamma_k(0) = P_{N_k,k}$ of the density matrix $\gamma(0)$ are smooth on each $\mathcal{B}_n$, and have discontinuities on the sheets $\mathcal{S}_n$.

Assumption 2.6 (semimetal)**.** *The dimension d is equal to 2, there is N_{sm} such that $\lambda_{N_{\text{sm}},k} \leq \mu_F$ for all $k \in \mathcal{B}$, and the Fermi surface $\mathcal{S}$ consists of a finite number of isolated points $(k_i)_{i\in\mathcal{I}}$ ("Dirac points"). All these points are conical crossings: for all $i \in \mathcal{I}$,*

$$\lambda_{N_{\text{sm}}-1,k_i} < \lambda_{N_{\text{sm}},k_i} = \mu_{\text{F}} = \lambda_{N_{\text{sm}}+1,k_i} < \lambda_{N_{\text{sm}}+2,k_i}, \tag{33}$$

$$\lambda_{N_{\text{sm}},k} = \mu_{\text{F}} - v_{F,i}|k-k_i| + O(|k-k_i|^2), \tag{34}$$

$$\lambda_{N_{\text{sm}}+1,k} = \mu_{\text{F}} + v_{F,i}|k-k_i| + O(|k-k_i|^2), \tag{35}$$

for some $v_{F,i} \in \mathbb{R}$. Furthermore, in this case we assume that $\mathcal{A} = 0$, so that the system has the time-reversal symmetry $H_{-k} = \overline{H_k}$.

Note that we assumed in Assumption 2.6 that $\mathcal{A} = 0$ to ensure time-reversal symmetry. We require more regularity on V than in the previous assumptions to be able to prove a Dyson expansion for the propagator (see Proposition 5.7). For the sake of clarity, we consider a model of 2D semimetals set in $\mathbb{R}^2$, but our arguments can be adapted to the more physical case of a model set in $\mathbb{R}^3$ (see also Remark 2.3).

Assumption 2.6 is generic in the case of potentials possessing the symmetry of honeycomb lattices, such as graphene [10]. In this case, there are two non-equivalent Dirac points in the Brillouin zone ($|\mathcal{I}| = 2$), usually denoted by K and K', and we have $K' = -K$ and $v_{F,1} = v_{F,2}$. The constant $v_F = v_{F,1} = v_{F,2}$ is known as the Fermi velocity. More generally, Dirac points generate specific dynamical behaviors that have been studied in [11, 14] in the context of the Dirac operator. Such phenomena also appear in molecular dynamics (see [19, 13, 12]).

In the semimetal case, $N_k = N_{\text{sm}}$ for almost every $k \in \mathbb{R}^2$, and $\gamma_k(0)$ is singular at each $k_i \in \mathcal{S}$.

2.5 Main results: the current

In the following results, we use the notation $O(f(\varepsilon,t))$ to denote a quantity bounded by $Cf(\varepsilon,t)$ where C is a constant that might depend on the material through V, $\mathcal{A}$ and μ_F, but not on t and ε.

Theorem 2.7 (insulators)**.** *Assume the system is an insulator (Assumption 2.4). Then there exists $\eta > 0$ such that for all $\varepsilon, t \in \mathbb{R}_+$,*

$$\frac{1}{t}\int_0^t \frac{j^\varepsilon_{\alpha,\beta}(t')}{\varepsilon}dt' = -i(2\pi)^{-d}\int_{\mathcal{B}} \mathrm{Tr}\left(\gamma_k(0)[\partial_\alpha\gamma_k(0),\partial_\beta\gamma_k(0)]\right)dk + O\left(\left(\frac{1}{t}+\varepsilon(1+t)\right)\mathrm{e}^{\eta\varepsilon t}\right).$$

Note that this implies in particular that

$$\sigma_{\alpha,\beta} = \lim_{t\to\infty}\frac{1}{t}\int_0^t \lim_{\varepsilon\to 0}\frac{j^\varepsilon_{\alpha,\beta}(t')}{\varepsilon}dt' = e_\alpha^T\sigma^\perp e_\beta,$$

where $\sigma^\perp$ is a real antisymmetric matrix with components

$$\sigma^\perp_{ij} := (2\pi)^{-d}\int_{\mathcal{B}} -i\,\mathrm{Tr}\left(\gamma_k(0)\left[\frac{\partial\gamma_k}{\partial k_i}(0),\frac{\partial\gamma_k}{\partial k_j}(0)\right]\right)dk. \tag{36}$$

The integrand in (36) is related to the well-known Berry curvature associated to the first N_{ins} bands, that is to the 2-form

$$\sum_{1\le i<j\le d}\Omega_{ij}(k)\,dk_i\wedge dk_j \quad \text{where} \quad \Omega_{ij} := -i\,\mathrm{Tr}\left(\gamma_k(0)\left[\frac{\partial\gamma_k}{\partial k_i}(0),\frac{\partial\gamma_k}{\partial k_j}(0)\right]\right)$$

For $d=2$, we have

$$\sigma^\perp_{12} = (2\pi)^{-1}\mathrm{Ch}_1(\gamma_\bullet(0)),$$

where $\mathrm{Ch}_1(\gamma_\bullet(0)) \in \mathbb{Z}$ is the first Chern of the fiber bundle defined by the quasi-periodic function $k \mapsto \gamma_k(0)$ [38, 34]. This relationship between the transverse bulk transport properties and the Chern number, characteristic of the integer quantum Hall effect, is known as the TKNN formula.

If $\mathcal{A}=0$, then the system has the time-reversal symmetry $H_{-k} = \overline{H_k}$. As is classical, the Berry curvature is then odd, and the transverse conductivity matrix $\sigma^\perp$ equal to zero [38].

Theorem 2.8 (conductivity in non-degenerate metals)**.** *Assume the system is a non-degenerate metal (Assumption 2.5).*

1. *Let $\theta > 0$. For all $\varepsilon > 0$ small enough and $0 \le t \le \frac{1}{\varepsilon}\varepsilon^\theta$, we have*

$$j^\varepsilon_{\alpha,\beta}(t) = D_{\alpha,\beta}\varepsilon t + O(\varepsilon+\varepsilon^2t^2) \tag{37}$$

where

$$D_{\alpha,\beta} := (2\pi)^{-d}\sum_{n\in\mathbb{N}^*}\int_{\mathcal{S}_n}\partial_\alpha\lambda_{n,k}\,(ds\cdot e_\beta) \tag{38}$$

2. *If furthermore there exists $N_{\mathrm{met}} \in \mathbb{N}^*$ such that $\lambda_{N_{\mathrm{met}}-1,k} < \mu_{\mathrm{F}} < \lambda_{N_{\mathrm{met}}+1,k}$ for all $k \in \mathcal{B}$ and there are uniform gaps between $\lambda_{N_{\mathrm{met}}-1,k}$ and $\lambda_{N_{\mathrm{met}},k}$ on the one hand, and $\lambda_{N_{\mathrm{met}},k}$ and $\lambda_{N_{\mathrm{met}}+1,k}$ on the other hand, then there exists $\eta > 0$ such that, for all $\varepsilon, t \in \mathbb{R}_+$,*

$$j^\varepsilon_{\alpha,\beta}(t) = -(2\pi)^{-d}\int_{\mathcal{B}}\mathbb{1}(\lambda_{N_{\mathrm{met}},k}\le\mu_{\mathrm{F}})\partial_\alpha\lambda_{N_{\mathrm{met}},k+\varepsilon e_\beta t}dk + O((\varepsilon+\varepsilon^2 t)\mathrm{e}^{\eta\varepsilon t}). \tag{39}$$

Note that under the assumptions of the case 2 above, the lowest $N-1$ bands are completely filled, the N^{th} band is partially filled, and the other bands are empty. Still in the setup of case 2, it follows from (37) and (39) that four different regimes can be observed for $\varepsilon \ll 1$

1. For very short times $t \ll 1$, quantum fluctuations of order $O(\varepsilon)$ dominate the current:

$$j^\varepsilon_{\alpha,\beta}(t) = O(\varepsilon);$$

2. For $1 \ll t \ll \frac{1}{\varepsilon}$, the electrons undergo ballistic transport:

$$j^\varepsilon_{\alpha,\beta}(t) \approx D_{\alpha,\beta}\varepsilon t,$$

where $D_{\alpha,\beta}$ is defined in (38);

3. For $\frac{1}{\varepsilon} \ll t \ll \frac{1}{\varepsilon}\log\big(\varepsilon^{-\zeta}\big)$ with $\zeta \in (0, \eta^{-1})$, we observe Bloch oscillations

$$j^{\varepsilon}_{\alpha,\beta}(t) \approx -(2\pi)^{-d} \int_{\mathcal{B}} \mathbb{1}(\lambda_{N_{\mathrm{met}},k} \leq \mu_{\mathrm{F}}) \partial_\alpha \lambda_{N_{\mathrm{met}},k+\varepsilon e_\beta t}\, dk.$$

   In particular, when e_β is commensurate with the reciprocal lattice $\mathcal{R}^*$, the current is well approximated in this regime by a periodic function of time with zero mean;

4. for times $t \gg \frac{1}{\varepsilon}\log\big(\varepsilon^{-\zeta}\big)$, our estimates do not allow us to conclude. The proofs show that the factor $\mathrm{e}^{\eta\varepsilon t}$ is due to the unboundedness of the operator H defined in (1). For tight-binding models, this factor $\mathrm{e}^{\eta\varepsilon t}$ is not present, and we would observe Bloch oscillations up to times $t \ll \frac{1}{\varepsilon^2}$. The behavior for larger times is open.

Note that some periodic metallic systems have a more complex crossing structure than that assumed in the second case of Theorem 2.8. This is the case in particular for the free electron gas ($V = 0$, $\mathcal{A} = 0$, seen as a periodic system with an arbitrary periodic lattice), which does not display Bloch oscillations.

Remark 2.9. The coherent electronic transport model considered here neglects all sources of dissipation (phonons, impurities, electron-electron interactions). In the Drude approximation, these phenomena give rise to an effective timescale τ such that $1 \ll \tau \ll 1/\varepsilon$ (larger than the coherence timescale of the electrons, but smaller than the Bloch oscillations timescale), yielding a finite DC conductivity $\sigma_{\alpha,\beta} \sim D_{\alpha,\beta}\tau$. In usual metals at room temperature, dissipation is dominated by phonon scattering, and the relaxation time τ is of the order of tens of femtoseconds [17]. By contrast, the timescale of Bloch oscillations in most experiments is much larger. Only in structures such as semiconductor superlattices or cold atoms have Bloch oscillations been observed experimentally [25].

Theorem 2.10 (conductivity in semi-metals)**.** *Assume that the system is a semimetal (Assumption 2.6). Assume furthermore that $V \in H^1_{\mathrm{per}}$. Then,*

$$\sigma_{\alpha,\beta} = \lim_{t\to\infty} \frac{1}{t} \int_0^t \lim_{\varepsilon\to 0} \frac{j^{\varepsilon}_{\alpha,\beta}(t')}{\varepsilon} dt' = \frac{|\mathcal{I}|}{16}\, e_\alpha \cdot e_\beta.$$

Semimetals are intermediate between insulators and metals, possessing a finite longitudinal conductivity in the linear response regime. This is due to the peculiar properties of the Dirac points. Note that the value of the conductivity is universal, not depending on the characteristics of the Hamiltonian but only on the number of conical crossings. More precisely, the conductivity tensor is isotropic and each conical intersection contributes as $\frac{1}{16}$ to the total conductivity. Note that this result is consistent with formula (1.17a) in [8].

3 Numerics

Before turning to the proofs, we illustrate our results with numerical simulations. As mentioned in Remark 2.3, our results also apply to tight-binding models, and only depend on the form of H_k. We test on a very simple model of H_k, adapted from the Haldane model [20] (itself based on a tight-binding model of graphene), that can support many phases depending on the values of its parameters. The graphene lattice $\mathcal{R}$ is spanned by the vectors

$$a_1 = \left(\frac{\sqrt{3}}{2}, \frac{1}{2}\right), \quad a_2 = \left(\frac{\sqrt{3}}{2}, -\frac{1}{2}\right),$$

and $\mathcal{R}^*$ by the vectors

$$b_1 = 2\pi\left(\frac{1}{\sqrt{3}}, 1\right), \quad b_2 = 2\pi\left(\frac{1}{\sqrt{3}}, -1\right).$$

The Hamiltonian fibers are

$$H_k = \begin{pmatrix} m(k) & \overline{f(k)} \\ f(k) & -m(k) \end{pmatrix},$$

with

$$m(k) = g + 2t_2\Big(\sin(k\cdot a_1) + \sin(k\cdot a_2) + \sin(k\cdot(a_1 - a_2))\Big),$$

$$f(k) = \sum_{i=1}^{3} \mathrm{e}^{ik\cdot\delta_i},$$

$$\delta_1 = \left(\frac{1}{\sqrt{3}}, 0\right), \quad \delta_2 = \left(-\frac{1}{2\sqrt{3}}, \frac{1}{2}\right), \quad \delta_3 = \left(-\frac{1}{2\sqrt{3}}, -\frac{1}{2}\right).$$

The eigenvalues of H_k are $\lambda_\pm = \pm\sqrt{m(k)^2 + |f(k)|^2}$. With $g = 0$, $t_2 = 0$, this is the standard model of graphene: two bands touching at level 0 at two inequivalent points in the Brillouin zone, where $f(k)$ vanishes. The parameter $g \neq 0$ opens a gap of size $2g$. The parameter t_2 models an internal magnetic field, and can turn the system into a Chern insulator (in particular, with $g = 1, t_2 = -1$, the system is a Chern insulator with Chern number $+1$). Therefore, varying the parameters g, t_2 and μ_{F}, we can obtain a normal insulator, a Chern insulator, a semimetal or a metal.

For a given set of parameters, we compute the current by using formulae (29)-(31). We sample the Brillouin zone using a uniform grid with $N_{\text{grid}} = 300$ points per direction, and solve the ordinary differential equation

$$i\frac{du}{dt}(t) = H_{k-\varepsilon e_\beta t}u(t), \quad u(0) = u_{n,k},$$

for various n and k using the `DifferentialEquations.jl` Julia package [31] with the default Tsitouras method of order 5.

Our parameter values are collected in Table 1.

Panel	g	μ_{F}	t_2	Phase
(a)	1	0	0	Normal insulator
(b)	1	0	-1	Chern insulator
(c)	1	-2	0	Metal
(d)	0	0	0	Semimetal

Table 1: Parameter values for the experiments in Figure 2

Our results are presented in the linear response regime ($\varepsilon = 10^{-6}$, $t \ll \frac{1}{\varepsilon}$) in Figure 2.

These results are consistent with our theoretical results, including the limit values of the conductivity in cases (b) and (d), where we obtain $4\pi/\sqrt{3} \approx 7.26$ and $|b_1|^2/8 = 2\pi^2/3 \approx 6.58$ respectively. However, there is an additional phenomenon worth of note: in the case of insulators and graphene, the linear response instantaneous conductivity $j_{\alpha,\beta}(t) = \lim_{\varepsilon\to 0} \frac{j^\varepsilon_{\alpha,\beta}(t)}{\varepsilon}$ seems to possess a finite limit as $t \to +\infty$. This is not captured by our results, where we used an averaging process to suppress the oscillations. Note that for a finite N_{grid}, the linear response oscillates with frequencies $\lambda_{n',k} - \lambda_{n,k}$ for $\lambda_{n,k} < \mu_{\mathrm{F}} < \lambda_{n',k}$, and k in the discrete Brillouin zone. Only in the limit $N_{\text{grid}} \to \infty$ do these resonances merge together to yield a finite limit for the current. This is linked to the absence of resonances (parallel bands) in our model. A deeper investigation of this effect would be interesting future work.

We also investigate the Bloch oscillations regime $\varepsilon \ll 1$, $\frac{1}{\varepsilon} \ll t$ in Figure 3, where we use the same parameters as in case (c) above. The result is consistent with our theoretical result: periodic or quasi-periodic oscillations, depending on whether e_β is commensurate with the reciprocal lattice or not.

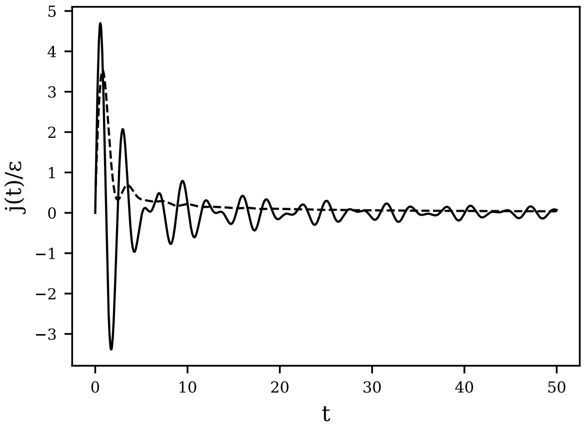
4 Bloch decomposition of $\gamma^\varepsilon_\beta(t)$ and regularity of the current

In this section, we prove Proposition 2.2. We first point out an alternative interpretation that helps shedding some light on the gauge change $G_{\varepsilon t e_\beta}$. Formally, $\gamma^\varepsilon_\beta(t)$ satisfies the equation

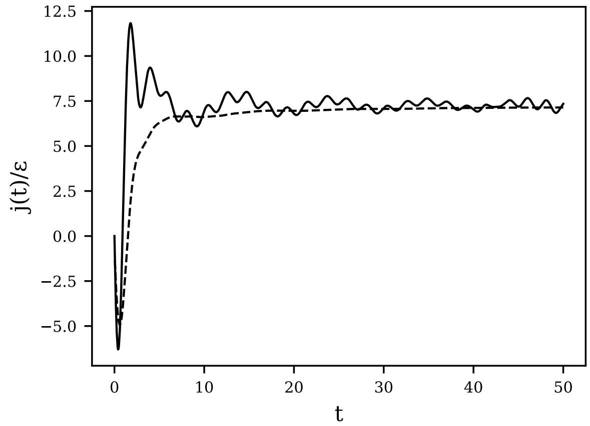
$$i\partial_t\gamma^\varepsilon_\beta = [H, \gamma^\varepsilon_\beta] + \varepsilon[x_\beta, \gamma^\varepsilon_\beta].$$

The operator $[x_\beta, \gamma^\varepsilon_\beta]$ can easily be seen to be $\mathcal{R}$-periodic, with fibers $i\partial_\beta\gamma^\varepsilon_{\beta,k}$ (where $\partial_\beta = e_\beta\cdot\nabla_k$), and therefore, $\gamma^\varepsilon_\beta(t)$ is $\mathcal{R}$-periodic and its fibers $\gamma^\varepsilon_{\beta,k}(t)$ satisfy the equation

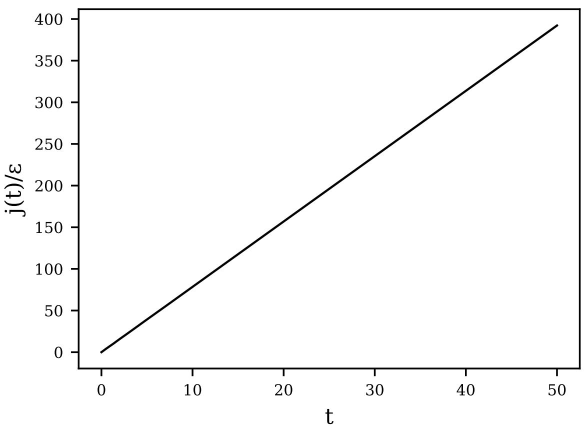
$$i\partial_t\gamma^\varepsilon_{\beta,k} - i\varepsilon\partial_\beta\gamma^\varepsilon_{\beta,k} = [H_k, \gamma^\varepsilon_{\beta,k}] = L_{H_k}\gamma^\varepsilon_{\beta,k},$$



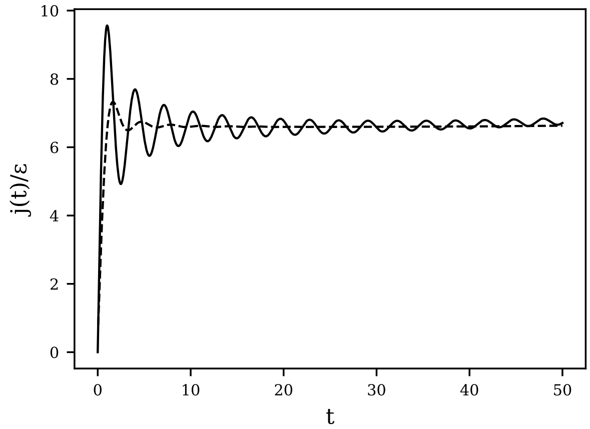
(a) Normal insulator phase, longitudinal current.



(b) Chern insulator phase, transverse current.



(c) Metallic phase.



(d) Graphene phase.

Figure 2: Instantaneous conductivity $\frac{j^{\varepsilon}_{\alpha,\beta}(t)}{\varepsilon}$ (solid line) and running average $\frac{1}{t}\int_0^t \frac{j^{\varepsilon}_{\alpha,\beta}(t')}{\varepsilon}dt'$ (dotted line) for several phases, in the linear response regime ($\varepsilon = 10^{-4}$, $t \ll \frac{1}{\varepsilon}$). In all cases $e_\beta = b_1$, and $e_\alpha = e_\beta$, except in panel (b) where $e_\alpha = b_2$.

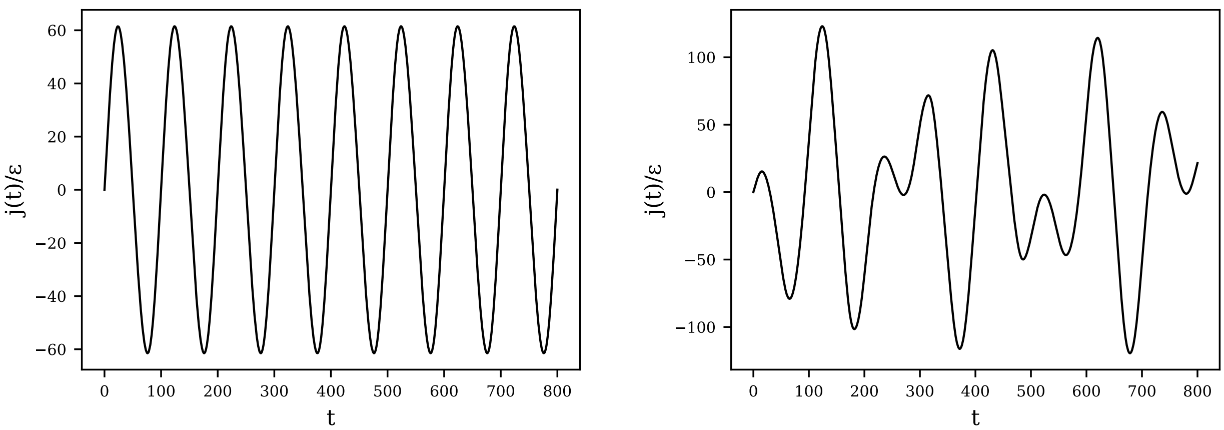


Figure 3: Instantaneous conductivity $\frac{j^{\varepsilon}_{\alpha,\beta}(t)}{\varepsilon}$ in the Bloch oscillations regime ($\varepsilon = 10^{-2}$, $\frac{1}{\varepsilon} \ll t$). We take $e_\alpha = b_1$. The left figure is with $e_\beta = b_1 + b_2$, the right one with $e_\beta = b_1 + \frac{1+\sqrt{5}}{2}b_2$.

where $L_{H_k} := [H_k, \cdot]$ is the Liouvillian associated with the operator H_k (see Section 5.1). The left-hand side of this equation is a linear advection equation, which suggests the use of the method of characteristics: setting

$$\widetilde{\gamma}^{\varepsilon}_{\beta,k}(t) = \gamma^{\varepsilon}_{\beta,k-\varepsilon e_\beta t}(t), \tag{40}$$

we obtain

$$i\partial_t \widetilde{\gamma}^{\varepsilon}_{\beta,k}(t) = [H_{k-\varepsilon e_\beta t}, \widetilde{\gamma}^{\varepsilon}_{\beta,k}(t)] = L_{H_{k-\varepsilon e_\beta t}} \widetilde{\gamma}^{\varepsilon}_{\beta,k}(t),$$

which is equivalent to (30). The use of the gauge transform operator $G_{\varepsilon t e_\beta}$, equivalent to the change of variable (40), makes these remarks rigorous.

We now prove Proposition 2.2. As outlined above, the results of this proposition are well-known; they can in fact be extended to the more general setting of ergodic magnetic Schrödinger operators (see [5]). We provide here an elementary proof specific to the periodic case, and take this opportunity to introduce notations and tools which will be useful in the sequel.

Proof of the first assertion. The essential self-adjointness of H^{ε}_{β} follows from an extension of the Faris-Lavine theorem [32, Theorem X.38]. Let $\mathcal{C} = C^{\infty}_{\mathrm{c}}(\mathbb{R}^d;\mathbb{C})$ be the set of infinitely differentiable, compactly supported functions.

Lemma 4.1 (Faris-Lavine theorem with periodic vector potentials)**.** *Let V and W be real-valued measurable functions on $\mathbb{R}^d$, $W \in L^2_{\mathrm{loc}}(\mathbb{R}^d;\mathbb{R})$ and $\mathcal{A} \in L^4_{\mathrm{per}}(\mathbb{R}^d;\mathbb{R}^d)$ such that $\nabla \cdot \mathcal{A} = 0$ in the sense of distributions. Suppose that*

1. *there exists $c, f \in \mathbb{R}_+$ such that $W(x) \geq -c|x|^2 - f$, for a.a. $x \in \mathbb{R}^d$;*
2. *$\frac{1}{2}(-i\nabla + \mathcal{A})^2 + V + W + 2c|x|^2$ is essentially self-adjoint on $\mathcal{C}$;*
3. *for some $a < 1$, $\frac{a}{2}(-i\nabla + \mathcal{A})^2 + V$ is bounded below on $\mathcal{C}$.*

Then $\frac{1}{2}(-i\nabla + \mathcal{A})^2 + V + W$ is essentially self-adjoint on $\mathcal{C}$.

The proof of the above lemma is postponed until Appendix A.1.

We apply Lemma 4.1 with $V \in L^2_{\mathrm{per}}(\mathbb{R}^d;\mathbb{R}), W = \varepsilon x_\beta$. The operator $\frac{1}{2}(-i\nabla + \mathcal{A})^2 + V + \varepsilon x_\beta + 2|x|^2$ is essentially self-adjoint on the core $\mathcal{C}$ in view of [24, Theorem 3] (note that $\varepsilon x \cdot e_\beta \geq -|x|^2 - \frac{\varepsilon^2 |e_\beta|^2}{4}$). Moreover, since V is $L^2_{\mathrm{per}}(\mathbb{R}^d;\mathbb{R})$, there exists $0 < a < 1$, such that $\frac{a}{2}(-i\nabla+\mathcal{A})^2+V$ is bounded below. This can be seen directly, or as a consequence of [24, Theorem 3]. Then, Lemma 4.1 gives that H^{ε}_{β} is essentially self-adjoint on $\mathcal{C}$ and therefore admits a unique self-adjoint extension on $L^2(\mathbb{R}^d;\mathbb{C})$. Hence, the propagator of the associated Schrödinger equation is well-defined, and explicitly given by $(\mathrm{e}^{-itH^{\varepsilon}_{\beta}})_{t\in\mathbb{R}}$.

Proof of the second assertion. The self-adjointness of the time-dependent Hamiltonian

$$\widetilde{H}^{\varepsilon}_{\beta}(t) = \frac{1}{2}(-i\nabla + \mathcal{A} - \varepsilon e_\beta t)^2 + V,$$

is a consequence of Lemma 4.1, by replacing $\mathcal{A}$ with $(\mathcal{A} - \varepsilon e_\beta t)$. To show the well-posedness of the dynamics, since $\widetilde{H}^{\varepsilon}_{\beta}(t)$ is $\mathcal{R}$-periodic, it suffices to study its fibers. Hence we consider the dynamics of a Schrödinger equation with Hamiltonian

$$\widetilde{H}^{\varepsilon}_{\beta,k}(t) = \frac{1}{2}(-i\nabla + \mathcal{A} + k - \varepsilon e_\beta t)^2 + V$$

and we use the following lemma on the dynamics generated by time-dependent perturbations of the free-particle Hamiltonian on L^2_{per}.

Lemma 4.2. *Let $H_0 := -\frac{1}{2}\Delta$ be the free-particle Hamiltonian on L^2_{per}, and a map*

$$[0, T] \ni t \mapsto H_1(t)$$

taking its values in the set of H_0-bounded self-adjoint operators on L^2_{per} with relative bound lower than 1, that is: there exist $0 < a < 1$ and $b > 0$ such that

$$\forall t \in [0, T], \quad \forall \phi \in H^2_{\mathrm{per}}, \quad \|H_1(t)\phi\|_{L^2_{\mathrm{per}}} \leq a\|H_0\phi\|_{L^2_{\mathrm{per}}} + b\|\phi\|_{L^2_{\mathrm{per}}}. \tag{41}$$

Then, for all $t \in [0, T]$, the operator defined by $H(t) = H_0 + H_1(t)$ is self-adjoint on L^2_{per} with domain H^2_{per}, and there exists a unique unitary propagator $(\mathcal{U}(t))_{t\in[0,T]}$ on L^2_{per} such that for $t \in [0, T]$, and $\phi_0 \in H^2_{\mathrm{per}}$, $\phi : t \mapsto \mathcal{U}(t)\phi_0$ is in $C^1([0, T]; H^2_{\mathrm{per}})$, and solves the time-dependent Schrödinger equation

$$i\partial_t \phi(t) = H(t)\phi(t), \qquad \phi(0) = \phi_0.$$

The proof of the above lemma is postponed to Appendix A.2.

For $t \in [0,T], k \in \mathbb{R}^d$, we have $\widetilde{H}^{\varepsilon}_{\beta,k}(t) = H_0 + H_1(t)$, with

$$H_1(t) = \frac{1}{2}\Big[(-i\nabla)\cdot(\mathcal{A}+k-\varepsilon e_\beta t) + (\mathcal{A}+k-\varepsilon e_\beta t)\cdot(-i\nabla) + (\mathcal{A}+k-\varepsilon e_\beta t)^2\Big] + V.$$

Using the Sobolev embeddings $H^2_{\rm per} \subset L^\infty_{\rm per}$, $H^1_{\rm per} \subset L^6_{\rm per}$ (recall that we assume $d \le 3$), the Coulomb gauge choice $\nabla\cdot\mathcal{A} = 0$ and the fact that $\mathcal{A} \in L^4_{\rm per}(\mathbb{R}^d;\mathbb{R}^d)$ and $V \in L^2_{\rm per}(\mathbb{R}^d;\mathbb{R})$, it is standard that H_1 satisfies the conditions of Lemma 4.2, and the result follows.

Proof of the third assertion. We first compute the fibers of the $\mathcal{R}$-periodic operator $\gamma^\varepsilon_\beta(t)$. Using (20), we have

$$\begin{aligned}
\gamma^\varepsilon_{\beta,k}(t) &= \left(G^*_{\varepsilon t e_\beta}\widetilde{\mathcal{U}}^\varepsilon_\beta(t)\gamma(0)\widetilde{\mathcal{U}}^\varepsilon_\beta(t)^* G_{\varepsilon t e_\beta}\right)_k &(42)\\
&= \left(\widetilde{\mathcal{U}}^\varepsilon_\beta(t)\gamma(0)\widetilde{\mathcal{U}}^\varepsilon_\beta(t)^*\right)_{k+\varepsilon t e_\beta}\\
&= \widetilde{\mathcal{U}}^\varepsilon_{\beta,k+\varepsilon t e_\beta}(t)\gamma_{k+\varepsilon t e_\beta}(0)\widetilde{\mathcal{U}}^\varepsilon_{\beta,k+\varepsilon t e_\beta}(t)^* &(43)\\
&= \sum_{n=1}^{N_{k+\varepsilon t e_\beta}} |\widetilde{\mathcal{U}}^\varepsilon_{\beta,k+\varepsilon t e_\beta}(t)u_{n,k+\varepsilon t e_\beta}\rangle\langle\widetilde{\mathcal{U}}^\varepsilon_{\beta,k+\varepsilon t e_\beta}(t)u_{n,k+\varepsilon t e_\beta}|.
\end{aligned}$$

Since the $u_{n,k}$ are in $H^2_{\rm per}$, we deduce that

$$(J_\alpha\gamma^\varepsilon_\beta(t))_k = -(-i\nabla+k+\mathcal{A})\cdot e_\alpha\gamma^\varepsilon_{\beta,k}(t) = -\partial_\alpha H_k\gamma^\varepsilon_{\beta,k}(t)$$

is trace-class (and finite-rank) uniformly in $k \in \mathcal{B}$ and therefore that the current $j^\varepsilon_{\alpha,\beta}(t) = \underline{\rm Tr}\left(J_\alpha\gamma^\varepsilon_\beta(t)\right)$ is well-defined.

As the function $k \mapsto {\rm Tr}\Big(\partial_\alpha H_k\gamma^\varepsilon_{\beta,k}(t)\Big)$ is $\mathcal{R}^*$-periodic, we also have

$$j^\varepsilon_{\alpha,\beta}(t) = -(2\pi)^{-d}\int_{\mathcal{B}} {\rm Tr}\big(\partial_\alpha H_k\gamma^\varepsilon_{\beta,k}(t)\big)\,dk = -(2\pi)^{-d}\int_{\mathcal{B}} {\rm Tr}\Big(\partial_\alpha H_{k-\varepsilon e_\beta t}\gamma^\varepsilon_{\beta,k-\varepsilon e_\beta t}(t)\Big)\,dk.$$

5 Perturbation theory for time-dependent Hamiltonians

In this section we consider the dynamics generated by a Hamiltonian $H(s) = H(\varepsilon t)$, and in particular its action on eigenspaces of $H(0)$. We begin with some elementary properties of the Liouvillian in Section 5.1, then use it to study subspace perturbation theory in Section 5.2. We establish an adiabatic theorem in Section 5.3, and use it to study the time-dependent Hamiltonian $H_{k-\varepsilon e_\beta t}$ in Section 5.4. Finally, we prove a result in linear response with a remainder independent of the gap in Section 5.5.

5.1 The Liouvillian and its partial inverse

In order to formulate and interpret our results, it is convenient to make use of the formalism of the Liouvillian and its partial inverse, a classical tool in adiabatic theory and eigenvalue perturbation theory [36, 21], although sometimes used implicitly. This formalism was for instance used in the context of transport properties in [1, 37, 28]. Recall that if h is a bounded self-adjoint operator on a Hilbert space $\mathcal{H}_{\rm f}$, the Liouvillian L_h associated with h is the bounded linear operator on $\mathcal{L}(\mathcal{H}_{\rm f})$ (such a mathematical object is sometimes called a superoperator in the physics literature) defined by

$$\forall A \in \mathcal{L}(\mathcal{H}_{\rm f}), \quad L_h A = [h, A]. \tag{44}$$

Note that if A is self-adjoint, then $L_h A$ is anti-self-adjoint ($iL_h A = i[h,A]$ is self-adjoint). The restriction of L_h to the space $\mathfrak{S}_2(\mathcal{H}_{\rm f})$ of Hilbert-Schmidt operators on $\mathcal{H}_{\rm f}$ is self-adjoint: for all $A, B \in \mathfrak{S}_2(\mathcal{H}_{\rm f})$,

$$(L_h A, B)_{\mathfrak{S}_2} = {\rm Tr}\left([h,A]^*B\right) = {\rm Tr}\left((A^*h - hA^*)B\right) = {\rm Tr}\left(A^*(hB-Bh)\right) = (A, L_h B)_{\mathfrak{S}_2}. \tag{45}$$

The operator L_h is to density matrices what the Hamiltonian h is to pure states: it is the infinitesimal generator of the norm-continuous unitary group $(\mathfrak{U}_h(t))_{t\in\mathbb{R}}$ on $\mathcal{L}(\mathcal{H}_{\rm f})$ defined by

$$\forall A \in \mathcal{L}(\mathcal{H}_{\rm f}), \quad \mathfrak{U}_h(t)A = e^{-ith}Ae^{ith}. \tag{46}$$

In the case when h is an unbounded self-adjoint operator, (44) does not make sense for all $A \in \mathcal{L}(\mathcal{H}_\mathrm{f})$, but it is still possible to define the Liouvillian L_h as the infinitesimal generator of the strongly-continuous unitary group $(\mathfrak{U}_h(t))_{t\in\mathbb{R}}$ on $\mathcal{L}(\mathcal{H}_\mathrm{f})$ defined by (46). It is then an unbounded operator on $\mathcal{L}(\mathcal{H}_\mathrm{f})$, self-adjoint on $\mathfrak{S}_2(\mathcal{H}_\mathrm{f})$.

If $\mathcal{H}_f$ is of finite-dimension N_f, the action of L_h is easily understood in an orthonormal eigenbasis $(e_n)_{1\le n\le N_f}$ of h with associated eigenvalues $\lambda_1 \le \cdots \le \lambda_{N_f}$. Then,

$$L_h|e_n\rangle\langle e_m| = (\lambda_n - \lambda_m)|e_n\rangle\langle e_m|.$$

The operator L_h is not invertible (for instance, $L_h|e_n\rangle\langle e_n| = 0$). However, it is invertible when restricted to the subspace of block off-diagonal matrices, i.e. matrices A such that $A_{nn'} = A_{mm'} = 0$ for $n, n' \le N < m, m'$ for a given N such that $\lambda_{N+1} > \lambda_N$. Its partial inverse $L^+_{h,N}$ is given by

$$\begin{aligned} L^+_{h,N}\Big(\sum_{1\le n\le N,\, N<m\le N_f} A_{mn}|e_m\rangle\langle e_n| + A_{nm}|e_n\rangle\langle e_m|\Big) \\ = \Big(\sum_{1\le n\le N,\, N<m\le N_f} \frac{A_{mn}|e_m\rangle\langle e_n| - A_{nm}|e_n\rangle\langle e_m|}{\lambda_m - \lambda_n}\Big) \end{aligned} \tag{47}$$

and $L^+_{h,N}$ is bounded in operator norm by $\frac{1}{\lambda_{N+1}-\lambda_N}$.

More generally, if h is an unbounded self-adjoint operator, let I be a closed bounded interval of $\mathbb{R}$, and assume that

$$g := \min\left(1, \mathrm{dist}\left(I, \sigma(h) \setminus (\sigma(h)\cap I)\right)\right) > 0.$$

The associated spectral projector is

$$P_{I,h} := \mathbb{1}_I(h) = \frac{1}{2\pi i}\oint_{\mathcal{C}} (z-h)^{-1}\, dz, \tag{48}$$

where $\mathcal{C}$ is a Cauchy contour in the complex plane such that $\sigma(h)\cap I$ is inside $\mathcal{C}$ and $\sigma(h)\setminus(\sigma(h)\cap I)$ is outside $\mathcal{C}$. Generalizing the terminology of the finite-dimensional case, we call off-diagonal operators (with respect to the splitting of $\mathcal{H}_f$ induced by $P_{I,h}$) the elements of the closed subspace

$$\mathcal{L}^{\mathrm{OD}}_{h,I} := \{A \in \mathcal{L}(\mathcal{H}_\mathrm{f}) \mid P_{h,I}AP_{h,I} = (1-P_{h,I})A(1-P_{h,I}) = 0\}$$

of $\mathcal{L}(\mathcal{H}_\mathrm{f})$. This defines a $\mathfrak{S}_2$-orthogonal splitting of operators into their diagonal and off-diagonal parts. It is easily seen that $\mathcal{L}^{\mathrm{OD}}_{h,I}$ is L_h-stable, and that L_h is invertible on $\mathcal{L}^{\mathrm{OD}}_{h,I}$ with a bounded inverse. We denote its partial inverse by $L^+_{h,I}$, extended to all of $\mathcal{L}(\mathcal{H}_f)$ by imposing that it vanishes on diagonal operators. We then have

$$L_{h,I}L^+_{h,I}A = L^+_{h,I}L_{h,I}A = P_{h,I}A(1-P_{h,I}) + (1-P_{h,I})AP_{h,I}$$

for all $A \in \mathcal{L}(\mathcal{H}_f)$.

It is easy to check that $L^+_{h,I}$ has an explicit contour integral representation:

$$L^+_{h,I}A = \frac{1}{2\pi i}\oint_{\mathcal{C}} (z-h)^{-1}[P_{h,I}, A](z-h)^{-1}\, dz, \quad \forall A \in \mathcal{L}(\mathcal{H}_\mathrm{f}), \tag{49}$$

where $\mathcal{C}$ is a contour as above. From (49), we see that, when $P_{h,I}$ is of finite rank $\mathcal{N}$, $L^+_{h,I}A$ is of rank of most $2\mathcal{N}$.

5.2 Subspace perturbation theory

The Liouvillian is a powerful tool to write concisely the results of subspace perturbation theory, which studies the time dependence of a gapped subspace of a time-dependent Hamiltonian. We consider $T > 0$ and $(H(s))_{s\in[0,T)}$ a family of self-adjoint operators on a Hilbert space $\mathcal{H}_\mathrm{f}$ sharing the same domain $D \subset \mathcal{H}_f$ and satisfying the following assumptions:

H1 $H(s) \ge 1$ for all $s \in [0,T)$;

H2 for each $\phi \in D$, the map $s \mapsto H(s)\phi$ is in $C^n([0,T), \mathcal{H}_\mathrm{f})$ for some $n \ge 1$. For all $1 \le l \le n$, the operator $H^{(l)}(s)$ is self-adjoint on $\mathcal{H}_\mathrm{f}$ for all $s \in [0,T)$, and

$$\alpha_l := \sup_{s\in[0,T)} \|H^{(l)}(s)H(s)^{-1}\|_{\mathcal{L}(\mathcal{H}_\mathrm{f})} < \infty; \tag{50}$$

H3 there exist $M \in \mathbb{R}_+$ and bounded continuous functions $a_\pm : [0,T] \to \mathbb{R}$ with $0 \le a_- \le a_+ \le M$ defining bounded closed intervals $I(s) = [a_-(s), a_+(s)] \subset \mathbb{R}$ such that, for all $s \in [0,T)$,

$$g(s) := \min\left(1, \operatorname{dist}(I(s), \sigma(H(s)) \setminus (\sigma(H(s)) \cap I(s)))\right) > 0,$$
$$P(s) := \mathbb{1}_{I(s)}(H(s)) \text{ has a finite (constant) rank } \mathcal{N} \in \mathbb{N}^*,$$

Under these assumptions, we set

$$L^+(s) := L^+_{H(s),I(s)}.$$

Proposition 5.1. *Assume* **H1**, **H2** *and* **H3**. *Then,* $P \in C^n([0,T), \mathcal{L}(\mathcal{H}_\mathrm{f}))$, $L^+ \in C^n([0,T), \mathcal{L}(\mathcal{L}(\mathcal{H}_\mathrm{f})))$, *and*

$$\dot{P}(s) = L(s)^+[P(s), \dot{H}(s)]. \tag{51}$$

Furthermore, there exist constants $C_1, \cdots, C_n \in \mathbb{R}_+$ *depending only on* $\alpha_1, \cdots, \alpha_n$ *and* M *such that the following bounds hold for all* $0 \le l \le n$, $s \in [0,T)$ *and* $A \in \mathcal{L}(\mathcal{H}_\mathrm{f})$:

$$\|H(s)P(s)\| \le M, \tag{52}$$
$$\|H(s)P^{(l)}(s)\| \le \frac{C_l}{g(s)^{l+1}}, \tag{53}$$
$$\|H(s)(L^+)^{(l)}(s)A\| \le \frac{C_l}{g(s)^{l+3}}\|A\|. \tag{54}$$

In addition, $P^{(l)}(s)$ *has rank at most* $(l+1)\mathcal{N}$, *and* $(L^+)^{(l)}(s)A$ *has rank at most* $c_l\mathcal{N}$ *where* c_l *is a constant that only depends on* l *(in particular,* $c_0 = 2$ *and* $c_1 = 10$*).*

Remark 5.2. The powers of the gap in the bounds (53) and (54) are too pessimistic, as could be shown by a more detailed analysis. For instance, in the case $l = 0$, $L^+(s)$ can be seen from the arguments at the beginning of this section to be bounded by a constant times $\frac{1}{g(s)}$. Similarly, the operator $\dot{P}$ is bounded by a constant times $\frac{1}{g(s)}$, using (51). Nevertheless, the above bounds are more straightforward to establish and will suffice for our purposes.

Proof. Differentiating $L_{H(s)}P(s) = 0$, we get

$$L_{H(s)}\dot{P}(s) = [P(s), \dot{H}(s)].$$

Since both $[P(s), \dot{H}(s)]$ and $\dot{P}(s)$ are off-diagonal operators (the first by direct calculation, the second by differentiating the relationship $P(s)^2 = P(s)$), we deduce (51). By the functional calculus, $\|H(s)P(s)\| = \|H(s)\mathbb{1}_{I(s)}(H(s))\| \le a_+(s) \le M$, whence (52).

In the following we take for $\mathcal{C}(s)$ the rectangular contour centered at the center of $I(s)$, of length $|I(s)| + g(s)$ and height $g(s)$, so that

$$|\mathcal{C}(s)| \le 2M + 4 \quad \text{and for all } z \in \mathcal{C}(s), \quad \left\|\frac{1}{z - H(s)}\right\| \le \frac{2}{g(s)}. \tag{55}$$

We use the integral representation (48):

$$P(s) = \frac{1}{2\pi i}\oint_{\mathcal{C}(s)} \frac{1}{z - H(s)}\, dz. \tag{56}$$

Using for all $z \in \mathcal{C}(s)$ the bound

$$\left\|\frac{H(s)}{z - H(s)}\right\| = \sup_{\lambda \in \sigma(H(s))}\left|\frac{\lambda}{z - \lambda}\right| \le 1 + \sup_{\lambda \in \sigma(H(s))}\left|\frac{z}{z - \lambda}\right| \le 1 + \frac{2(M + g(s))}{g(s)} \le \frac{2M+3}{g(s)} \tag{57}$$

establishes (53) for $l = 0$.

The contour $\mathcal{C}(s)$ in (56) above can be kept fixed equal to $\mathcal{C}(s_0)$ for s in a neighborhood of any $s_0 \in [0,T)$. Using

$$\frac{d}{ds}\frac{1}{z - H(s)} = \frac{1}{z - H(s)}\dot{H}(s)\frac{1}{z - H(s)} \tag{58}$$

it follows that $P \in C^1([0,T), \mathcal{L}(\mathcal{H}_\mathrm{f}))$ and

$$\dot{P}(s) = \frac{1}{2\pi i} \oint_{\mathcal{C}(s)} \frac{1}{z - H(s)} \dot{H}(s) \frac{1}{z - H(s)} \, dz.$$

Using the bounds (50), (55) and (57), it follows that

$$\|H(s)\dot{P}(s)\| \leq \frac{(2M+3)(2M+4)\alpha_1}{\pi g(s)^2}$$

which proves (53) for $l = 1$. The general case for $l > 1$ follows from repeated application of the chain rule to (56) and (58), and the bounds (50), (55) and (57).

The differentiability and bounds on the inverse Liouvillian are treated using the same arguments on the representation

$$L^+(s)A = \frac{1}{2\pi i} \oint_{\mathcal{C}(s)} \frac{1}{z - H(s)} [P(s), A] \frac{1}{z - H(s)} \, dz.$$

Let $(u_n^0)_{n=1,\dots,\mathcal{N}}$ be an orthonormal basis of $P(0)$. Then the solutions to the parallel transport equation $\dot{u}_n(s) = \dot{P}(s)u_n(s)$ with $u_n(0) = u_n^0$ are easily checked to be a C^n orthogonal basis of $\mathrm{Ran}P(s)$. It follows that one has

$$P^{(l)}(s) = \sum_{n=1}^{\mathcal{N}} \sum_{m=0}^{l} \binom{l}{m} |u_n^{(m)}(s)\rangle\langle u_n^{(l-m)}(s)|.$$

Therefore, $P^{(l)}(s)$ is of rank at most $(l+1)\mathcal{N}$. From the integral representation of $L^+(s)$ (see (49)), it follows that, for any bounded operator A, $L^+(s)A$ is of rank at most $2\mathcal{N}$. Its derivatives are sums of terms which all contain as a factor $P(s)$ or one of its derivative, and the result follows with $c_l = 2 \sum_{k_1+k_2+k_3=l,\, k_j \in \mathbb{N}} (k_2+1)$. $\square$

5.3 Adiabatic theory

The following proposition is an adaptation in our context of the classical adiabatic theorem that the Schrödinger evolution with a slowly evolving Hamiltonian $H(\varepsilon t)$ approximately preserves gapped eigenspaces [36]. We explicitly compute the corrections to first order in ε.

Proposition 5.3. *Assume the same hypotheses as in Proposition 5.1. Let $(U^\varepsilon(t,t'))_{0 \leq t' \leq t < \varepsilon^{-1}T}$ be the propagator associated with the family of time-scaled Hamiltonians $(H(\varepsilon t))_{t \in [0, \varepsilon^{-1}T)}$, i.e.*

$$i\frac{\partial U^\varepsilon}{\partial t}(t,t') = H(\varepsilon t)U^\varepsilon(t,t'), \quad t \in [t', \varepsilon^{-1}T) \qquad U^\varepsilon(t',t') = \mathrm{Id}, \tag{59}$$

and $U^\varepsilon(t) = U^\varepsilon(t,0)$. For all $\varepsilon \geq 0$ and $t \in [0, \varepsilon^{-1}T)$, it holds

$$U^\varepsilon(t)P(0)U^\varepsilon(t)^* = P(\varepsilon t) + i\varepsilon L^+(\varepsilon t)\dot{P}(\varepsilon t) - i\varepsilon U^\varepsilon(t)\left(L^+(0)\dot{P}(0)\right)U^\varepsilon(t)^* + R^\varepsilon(t), \tag{60}$$

with

$$R^\varepsilon(t) = -i\varepsilon^2 \int_0^t U^\varepsilon(t,t') \, \frac{d}{ds}\left(L(s)^{-1}\dot{P}(s)\right)\Big|_{s=\varepsilon t'} U^\varepsilon(t,t')^* \, dt'. \tag{61}$$

In addition, we have the following estimates:

$$\forall 0 \leq t' \leq t < \varepsilon^{-1}T, \quad \left\|H(\varepsilon t)U^\varepsilon(t,t')H(\varepsilon t')^{-1}\right\|_{\mathcal{L}(\mathcal{H}_\mathrm{f})} \leq e^{\alpha_1 \varepsilon (t-t')}, \tag{62}$$

$$\left\|H(\varepsilon t)^{1/2}U^\varepsilon(t,t')H(\varepsilon t')^{-1/2}\right\|_{\mathcal{L}(\mathcal{H}_\mathrm{f})} \leq e^{\alpha_1 \varepsilon (t-t')/2}. \tag{63}$$

Proof. The existence and uniqueness of the strongly-continuous unitary propagator $(U^\varepsilon(t,t'))$ satisfying (59) can be obtained using (50) for $l = 1$, and Theorem X.70 and the arguments in the proof of Theorem X.71 in [32]. We pass to the interaction picture defined by $H(\varepsilon t)$ and compute the evolution of a C^1 time-dependent Hilbert-Schmidt observable $A^\varepsilon(t)$ in that picture:

$$\frac{d}{dt}\left(U^\varepsilon(t)^* A^\varepsilon(t) U^\varepsilon(t)\right) = U^\varepsilon(t)^* \left(\dot{A}^\varepsilon(t) + i[H(\varepsilon t), A^\varepsilon(t)]\right) U^\varepsilon(t). \tag{64}$$

We first apply (64) to $A^\varepsilon(t) = P(\varepsilon t)$ and obtain

$$\frac{d}{dt}\left(U^\varepsilon(t)^* P(\varepsilon t) U^\varepsilon(t)\right) = \varepsilon\, U^\varepsilon(t)^* \dot{P}(\varepsilon t) U^\varepsilon(t). \tag{65}$$

Estimating this to be of size ε is not enough because we look at long time scales. What allows us to proceed further is that this quantity is oscillating on a timescale of order $O(1)$. Indeed, applying (64) to $A^\varepsilon(t) = L^+(\varepsilon t)\dot{P}(\varepsilon t)$, for which $[H(\varepsilon t), A^\varepsilon(t)] = \dot{P}(\varepsilon t)$, we obtain

$$U^\varepsilon(t)^* \dot{P}(\varepsilon t) U^\varepsilon(t) = -i\frac{d}{dt}\left(U^\varepsilon(t)^*(L^+(\varepsilon t)\dot{P}(\varepsilon t))U^\varepsilon(t)\right) + iU^\varepsilon(t)^* \frac{d}{dt}\left(L^+(\varepsilon t)\dot{P}(\varepsilon t)\right) U^\varepsilon(t).$$

Integrating (65) over $[0,t]$ and using the above equality leads to

$$\begin{aligned} U^\varepsilon(t)^* P(\varepsilon t) U^\varepsilon(t) &= P(0) + \varepsilon \int_0^t U^\varepsilon(t')^* \dot{P}(\varepsilon t') U^\varepsilon(t')\, dt' \\ &= P(0) - i\varepsilon U^\varepsilon(t)^* \left(L^+(\varepsilon t)\dot{P}(\varepsilon t)\right) U^\varepsilon(t) + i\varepsilon L^+(0)\dot{P}(0) + r^\varepsilon(t) \end{aligned}$$

with

$$r^\varepsilon(t) = i\varepsilon \int_0^t U^\varepsilon(t')^* \frac{d}{dt'}\left(L^+(\varepsilon t')\dot{P}(\varepsilon t')\right) U^\varepsilon(t')\, dt' = i\varepsilon^2 \int_0^t U^\varepsilon(t')^* \left.\frac{d}{ds}\left(L^+(s)\dot{P}(s)\right)\right|_{s=\varepsilon t'} U^\varepsilon(t')\, dt'.$$

This implies

$$U^\varepsilon(t) P(0) U^\varepsilon(t)^* = P(\varepsilon t) + i\varepsilon L^+(\varepsilon t)\dot{P}(\varepsilon t) - i\varepsilon U^\varepsilon(t)\left(L^+(0)\dot{P}(0)\right) U^\varepsilon(t)^* + R^\varepsilon(t), \tag{66}$$

with

$$R^\varepsilon(t) = -i\varepsilon^2 \int_0^t U^\varepsilon(t,t') \left.\frac{d}{ds}\left(L^+(s)\dot{P}(s)\right)\right|_{s=\varepsilon t'} U^\varepsilon(t,t')^*\, dt',$$

which establishes (60).

Let us now prove (62). Let $\psi \in D$. For all $t \in [t', \varepsilon^{-1}T)$, we set $\psi_\varepsilon(t) = U^\varepsilon(t,t')\psi$ and $\phi_\varepsilon(t) = H(\varepsilon t)\psi_\varepsilon(t)$. We have

$$i\frac{d\phi_\varepsilon}{dt}(t) = i\frac{d}{dt}\left(H(\varepsilon t)\psi_\varepsilon(t)\right) = H(\varepsilon t)\phi_\varepsilon(t) + i\varepsilon \dot{H}(\varepsilon t) H(\varepsilon t)^{-1}\phi_\varepsilon(t),$$

from which we obtain

$$\phi_\varepsilon(t) = U^\varepsilon(t,t')H(\varepsilon t')\psi + i\varepsilon \int_{t'}^t \dot{H}(\varepsilon t'')H(\varepsilon t'')^{-1}\phi_\varepsilon(t'')\, dt'',$$

and finally

$$\|\phi_\varepsilon(t)\|_{\mathcal{H}_\mathrm{f}} \le \|H(\varepsilon t')\psi\|_{\mathcal{H}_\mathrm{f}} + \alpha_1 \varepsilon \int_{t'}^t \|\phi_\varepsilon(t'')\|_{\mathcal{H}_\mathrm{f}}\, dt''.$$

By the Grönwall lemma,

$$\|H(\varepsilon t)U^\varepsilon(t,t')\psi\|_{\mathcal{H}_\mathrm{f}} = \|\phi_\varepsilon(t)\|_{\mathcal{H}_\mathrm{f}} \le \|H(\varepsilon t')\psi\|_{\mathcal{H}_\mathrm{f}} e^{\alpha_1 \varepsilon (t-t')}.$$

Applying this inequality to $\psi = H(\varepsilon t')^{-1}\phi$ for all $\phi \in \mathcal{H}_\mathrm{f}$ gives (62). We obtain (63) by interpolation (see e.g. [32, Section IX.4, Proposition 9]). □

The third term

$$-U^\varepsilon(t)\left(iL^+(0)\dot{P}(0)\right)U^\varepsilon(t)^*$$

of the right-hand side of (60) is oscillatory, and can be written as the derivative of a bounded function up to higher order terms. Its time-average therefore becomes negligible in the considered regimes. Let us introduce the space

$$\mathcal{L}^{\mathrm{OD}}(s) := \{A \in \mathcal{L}(\mathcal{H}_\mathrm{f}) \mid P(s)AP(s) = (1-P(s))A(1-P(s)) = 0\}$$

of bounded off-diagonal operators relatively to the decomposition $\mathcal{H}_\mathrm{f} = \mathrm{Ran}(P(s)) \oplus \mathrm{Ker}(P(s))$.

Lemma 5.4. *Under the assumptions of Propositions 5.1 and 5.3, we have for any self-adjoint operator $A \in \mathcal{L}^{\mathrm{OD}}(0)$,*

$$U^\varepsilon(t)AU^\varepsilon(t)^* = \frac{d}{dt}\left(iL^+(\varepsilon t)\left(U^\varepsilon(t)AU^\varepsilon(t)^*\right)\right) + R_A^\varepsilon(t), \tag{67}$$

where

$$R_A^\varepsilon(t) = 2U^\varepsilon(t)r^\varepsilon(t)Ar^\varepsilon(t)U^\varepsilon(t)^* - \Big(U^\varepsilon(t)(1-2P(0))Ar^\varepsilon(t)U^\varepsilon(t)^* + \text{h.c.}\Big) + \varepsilon i\frac{dL^+}{ds}(\varepsilon t)\Big(U^\varepsilon(t)AU^\varepsilon(t)^*\Big)$$

and

$$r^\varepsilon(t) = -i\varepsilon U^\varepsilon(t)^*\left(L^+(\varepsilon t)\dot{P}(\varepsilon t)\right)U^\varepsilon(t) + i\varepsilon L^+(0)\dot{P}(0) + U^\varepsilon(t)^* R^\varepsilon(t)U^\varepsilon(t).$$

Proof. We have

$$\begin{aligned}
\frac{d}{dt}\left(iL^+(\varepsilon t)\left(U^\varepsilon(t)AU^\varepsilon(t)^*\right)\right) &= \varepsilon i\frac{dL^+}{ds}(\varepsilon t)\left(U^\varepsilon(t)AU^\varepsilon(t)^*\right) + L^+(\varepsilon t)L(\varepsilon t)\left(U^\varepsilon(t)AU^\varepsilon(t)^*\right)\\
&= \varepsilon i\frac{dL^+}{ds}(\varepsilon t)U^\varepsilon(t)AU^\varepsilon(t)^* + P(\varepsilon t)U^\varepsilon(t)AU^\varepsilon(t)^*(1-P(\varepsilon t)) + \text{h.c.},
\end{aligned}$$

and we deduce from (60) that $P(\varepsilon t)U^\varepsilon(t) = U^\varepsilon(t)\left(P(0) + r^\varepsilon(t)\right)$. We therefore have

$$\begin{aligned}
P(\varepsilon t)U^\varepsilon(t)AU^\varepsilon(t)^*(1-P(\varepsilon t)) + \text{h.c.} =& U^\varepsilon(t)\left(P(0)+r^\varepsilon(t)\right)A(1-P(0)-r^\varepsilon(t))U^\varepsilon(t)^* + \text{h.c.}\\
=& U^\varepsilon(t)AU^\varepsilon(t)^* + \left(U^\varepsilon(t)\left(1-2P(0)\right)Ar^\varepsilon(t)U^\varepsilon(t)^* + \text{h.c.}\right)\\
&+ 2U^\varepsilon(t)r^\varepsilon(t)Ar^\varepsilon(t)U^\varepsilon(t)^*,
\end{aligned}$$

where we have used that $A = P(0)A(1-P(0)) + (1-P(0))AP(0)$. ☐

5.4 Application to coherent transport in Bloch representation

Let H be the periodic magnetic Hamiltonian defined in (1), J the current operator whose components are defined in (6), μ_{F} the Fermi level,

$$\mu := 1 + \min\sigma(H) \quad \text{and} \quad \eta = \max_{|e|\le|e_\alpha|,|e_\beta|}\|(J\cdot e)(H+\mu)^{-1}\|_{\mathcal{L}(L^2(\mathbb{R}^d;\mathbb{C}))} < \infty.$$

Let $k \in \mathbb{R}^d$. Assume that $\lambda_{N_k+1,k} - \lambda_{N_k,k} > 0$ and set

$$s_k = \inf\{s > 0 \,|\, g_k(s) = 0\} \quad \text{where} \quad g_k(s) := \min(1, \lambda_{N_k+1,k-se_\beta} - \lambda_{N_k,k-se_\beta}).$$

We consider the family of Hamiltonians

$$H(s) := H_{k-e_\beta s} + \mu. \tag{68}$$

We have

$$\dot{H}(s) = -\partial_\beta H_{k-se_\beta} = -((-i\nabla + k + \mathcal{A} - se_\beta)\cdot e_\beta) = J_{\beta,k-se_\beta}, \tag{69}$$

$$\ddot{H}(s) = |e_\beta|^2 \mathrm{Id}_{L^2_{\mathrm{per}}}, \tag{70}$$

and so hypotheses H1-H3 of Proposition 5.1 are satisfied with $\mathcal{H}_{\mathrm{f}} = L^2_{\mathrm{per}}$, $D = H^2_{\mathrm{per}}$, $T = s_k$, n arbitrarily large, $\alpha_1 \le \eta$, $\alpha_2 = |e_\beta|^2$, $\alpha_l = 0$ for $l \ge 3$, $a_-(s) = \min\sigma(H) + \mu$, $a_+(s) = \lambda_{N_k,k-se_\beta} + \mu$, $M = \max_{k'\in\mathcal{B}}\lambda_{N_{k'}+1,k'} + \mu$, $g(s) = g_k(s)$, and $\mathcal{N} = N_k$.

Corollary 5.5. *Let $k \in \mathbb{R}^d$ such that $\lambda_{N_k+1,k} - \lambda_{N_k,k} > 0$. Then, for all $\varepsilon > 0$ and $t \in [0, \varepsilon^{-1}s_k)$, the operator $\partial_\alpha H_{k-\varepsilon e_\beta t}\gamma^\varepsilon_{\beta,k-\varepsilon e_\beta t}(t)$ is in $\mathfrak{S}_{1,\mathrm{per}}$, and we have*

$$\begin{aligned}
\mathrm{Tr}(\partial_\alpha H_{k-\varepsilon e_\beta t}\widetilde{\mathcal{U}}^\varepsilon_{\beta,k}(t)\gamma_k(0)\widetilde{\mathcal{U}}^\varepsilon_{\beta,k}(t)^*) =& \partial_\alpha\left(\mathrm{Tr}\big(H_{k-\varepsilon e_\beta t}P_{N_k,k-\varepsilon e_\beta t}\big)\right)\\
&+ i\varepsilon\,\mathrm{Tr}\Big(\partial_\alpha H_{k-\varepsilon e_\beta t}L^+_{N_k,k-\varepsilon e_\beta t}\partial_\beta P_{N_k,k-\varepsilon e_\beta t}\Big)\\
&- i\varepsilon\,\mathrm{Tr}\Big(\partial_\alpha H_{k-\varepsilon e_\beta t}\widetilde{\mathcal{U}}^\varepsilon_{\beta,k}(t)\ L^+_{N_k,k}\partial_\beta P_{N_k,k}\widetilde{\mathcal{U}}^\varepsilon_{\beta,k}(t)^*\Big)\\
&+ \mathfrak{R}^\varepsilon_k(t),
\end{aligned} \tag{71}$$

where each term of the right-hand side is a well-defined real number and $L^+_{N,k}$ *is a shorthand notation for the inverse Liouvillian* $L^+_{H_k,[\lambda_{1,k},\lambda_{N,k}]}$. *In addition, we have the following bounds*

$$|\mathrm{Tr}(\partial_\alpha H_{k-\varepsilon e_\beta t}\widetilde{\mathcal{U}}^\varepsilon_{\beta,k}(t)\gamma_k(0)\widetilde{\mathcal{U}}^\varepsilon_{\beta,k}(t)^*)| \leq Ce^{\eta\varepsilon t}, \tag{72}$$

$$|\partial_\alpha\left(\mathrm{Tr}\big(H_{k-\varepsilon e_\beta t}P_{N_k,k-\varepsilon e_\beta t}\big)\right)| \leq C,$$

$$|\varepsilon\,\mathrm{Tr}\Big(\partial_\alpha H_{k-\varepsilon e_\beta t}L^+_{N_k,k-\varepsilon e_\beta t}\partial_\beta P_{N_k,k-\varepsilon e_\beta t}\Big)| \leq C\frac{\varepsilon}{g_k(\varepsilon t)^4},$$

$$|\varepsilon\,\mathrm{Tr}\Big(\partial_\alpha H_{k-\varepsilon e_\beta t}\widetilde{\mathcal{U}}^\varepsilon_{\beta,k}(t)\ L^+_{N_k,k}\partial_\beta P_{N_k,k}\widetilde{\mathcal{U}}^\varepsilon_{\beta,k}(t)^*\Big)| \leq C\frac{\varepsilon e^{\eta\varepsilon t}}{g_k(0)^4}, \tag{73}$$

$$|\mathfrak{R}^\varepsilon_k(t)| \leq \frac{C\varepsilon^2 te^{\eta\varepsilon t}}{\min_{s\in[0,\varepsilon t]} g_k(s)^6}, \tag{74}$$

for a constant $C \in \mathbb{R}_+$ *independent of* k, ε *and* t.

Proof. Applying the second assertion in Proposition 5.3, we get

$$\begin{aligned}\widetilde{\mathcal{U}}^\varepsilon_{\beta,k}(t)\gamma_k(0)\widetilde{\mathcal{U}}^\varepsilon_{\beta,k}(t)^* =& P_{N_k,k-\varepsilon e_\beta t} + i\varepsilon L^+_{N_k,k-\varepsilon e_\beta t}\partial_\beta P_{N_k,k-\varepsilon e_\beta t}\\ &- i\varepsilon\widetilde{\mathcal{U}}^\varepsilon_{\beta,k}(t)\ \left(L^+_{N_k,k}\partial_\beta P_{N_k,k}\right)\widetilde{\mathcal{U}}^\varepsilon_{\beta,k}(t)^* + R^\varepsilon_k(t).\end{aligned} \tag{75}$$

Each term A in (75) being a finite-rank self-adjoint operator, it holds

$$\|\partial_\alpha H_{k-\varepsilon e_\beta t}A\|_{\mathfrak{S}_1} \leq \mathrm{Rank}(A)\|\partial_\alpha H_{k-\varepsilon e_\beta t}A\| \leq \eta\mathrm{Rank}(A)\|(H_{k-\varepsilon e_\beta t}+\mu)A\|,$$

and again by Proposition 5.3 we get

$$\begin{aligned}\mathrm{Tr}(\partial_\alpha H_{k-\varepsilon e_\beta t}\widetilde{\mathcal{U}}^\varepsilon_{\beta,k}(t)\gamma_k(0)\widetilde{\mathcal{U}}^\varepsilon_{\beta,k}(t)^*) =& \mathrm{Tr}\big(\partial_\alpha H_{k-\varepsilon e_\beta t}P_{N_k,k-\varepsilon e_\beta t}\big)+i\varepsilon\,\mathrm{Tr}\Big(\partial_\alpha H_{k-\varepsilon e_\beta t}L^+_{N_k,k-\varepsilon e_\beta t}\partial_\beta P_{N_k,k-\varepsilon e_\beta t}\Big)\\ &-i\varepsilon\,\mathrm{Tr}\Big(\partial_\alpha H_{k-\varepsilon e_\beta t}\widetilde{\mathcal{U}}^\varepsilon_{\beta,k}(t)\ \left(L^+_{N_k,k}\partial_\beta P_{N_k,k}\right)\widetilde{\mathcal{U}}^\varepsilon_{\beta,k}(t)^*\Big) + \mathrm{Tr}\left(\partial_\alpha H_{k-\varepsilon e_\beta t}R^\varepsilon_k(t)\right)\end{aligned}$$

with

$$R^\varepsilon_k(t) = i\varepsilon^2\int_0^t \widetilde{\mathcal{U}}^\varepsilon_{\beta,k}(t,t')\partial_{k_\beta}\left(L^+_{N_k,k-\varepsilon e_\beta t'}\partial_{k_\beta}P_{N_k,k-\varepsilon e_\beta t'}\right)\widetilde{\mathcal{U}}^\varepsilon_{\beta,k}(t,t')^*\ dt'. \tag{76}$$

It results from the Hellmann-Feynman formula that

$$\mathrm{Tr}\big(\partial_\alpha H_{k-\varepsilon e_\beta t}P_{N,k-\varepsilon e_\beta t}\big) = \partial_\alpha\left(\mathrm{Tr}\big(H_{k-\varepsilon e_\beta t}P_{N,k-\varepsilon e_\beta t}\big)\right).$$

Finally, using Propositions 5.1 and 5.3, we obtain the bounds (72)-(74). In particular,

$$\begin{aligned}|\mathfrak{R}^\varepsilon_k(t)| &= \left|\mathrm{Tr}\left(\partial_\alpha H_{k-\varepsilon e_\beta t}R^\varepsilon_k(t)\right)\right|\\ &\leq 4N_k\varepsilon^2\eta t\sup_{t'\in[0,t)}\left(e^{\eta\varepsilon(t-t')}\left\|H_{k-\varepsilon e_\beta t'}\partial_{k_\beta}\left(L^+_{N_k,k-\varepsilon e_\beta t'}\partial_{k_\beta}P_{N_k,k-\varepsilon e_\beta t'}\right)\right\|\right)\\ &\leq C\frac{\eta\varepsilon^2 te^{\eta\varepsilon t}}{\inf_{s\in[0,\varepsilon t)} g_k(s)^6},\end{aligned}$$

where $C \in \mathbb{R}_+$ is independent of k, ε and t. □

Remark 5.6. The decomposition (71) will be key to computing the current in insulators, non-degenerate metals and semimetals. The first three terms in the right-hand side of (71) have different physical meanings. The first term is the adiabatic term: electrons simply are transported adiabatically across the Brillouin zone. This term will be responsible for the ballistic transport of electrons in metals. The second is the first-order static response, and will be the cause of the Hall conductivity in insulators. The third is oscillatory, and is related to the AC response of solids (not treated here). This decomposition only makes sense for a non-zero gap; in particular, it cannot be used to compute the contribution to the current for k points close to Dirac points for semimetals.

5.5 Linear response

We now aim at obtaining an expansion of the current to first order in ε for a given t, based on a Dyson expansion instead of the adiabatic theorem. This is a classical computation in response theory, sometimes known as the Kubo formula [22]. In contrast to the previous result, this gives a remainder that does not depend on a gap, and will therefore be useful for the study of semimetals near Dirac points.

Proposition 5.7. *Let H be the periodic magnetic Hamiltonian defined in (1). Under the additional assumptions that $V \in H^1_{\rm per}$ and $\mathcal{A} \in (H^2_{\rm per})^d$, there exists a constant $C \in \mathbb{R}_+$ such that for all $k \in \mathbb{R}^d$ such that $\lambda_{N_k+1,k} - \lambda_{N_k,k} > 0$, we have for all $\varepsilon, t \in \mathbb{R}_+$,*

$$\begin{aligned}\mathrm{Tr}\left(\partial_\alpha H_{k-\varepsilon e_\beta t}\widetilde{\mathcal{U}}^\varepsilon_{\beta,k}(t)\,\gamma_k(0)\,\widetilde{\mathcal{U}}^\varepsilon_{\beta,k}(t)^*\right) =&\partial_\alpha \mathrm{Tr}\left(H_k\gamma_k(0)\right) - \varepsilon t\partial_\alpha\partial_\beta\left(\mathrm{Tr}(H_k\gamma_k(0))\right)\\ &+ i\varepsilon\,\mathrm{Tr}\big(\partial_\alpha H_k(e^{-itL_k}-1)L_k^+\partial_\beta\gamma_k(0)\big) + \rho^\varepsilon_k(t),\end{aligned} \tag{77}$$

with, when $\varepsilon t \le 1$,

$$|\rho^\varepsilon_k(t)| \le C\varepsilon^2 t^3(1+t^3). \tag{78}$$

Proof. Let k be such that $\lambda_{N_k+1,k} - \lambda_{N_k,k} > 0$. Since $k' \mapsto \mathrm{Tr}\left(H_{k'}\gamma_{k'}(0)\right)$ is real-analytic in a neighborhood of k, we have by Hellmann-Feynman theorem

$$\partial_\alpha \mathrm{Tr}\left(H_k\gamma_k(0)\right) = \mathrm{Tr}\left(\partial_\alpha H_k\gamma_k(0)\right) \quad \text{and} \quad \partial_\alpha\partial_\beta \mathrm{Tr}\left(H_k\gamma_k(0)\right) = \mathrm{Tr}\left(\partial_\alpha\partial_\beta H_k\gamma_k(0)\right) + \mathrm{Tr}\left(\partial_\alpha H_k\partial_\beta\gamma_k(0)\right).$$

We also have $\partial_\alpha H_{k-\varepsilon e_\beta t} = \partial_\alpha H_k - \varepsilon t e_\alpha\cdot e_\beta$. It follows that

$$\begin{aligned}\rho^\varepsilon_k(t) =&\mathrm{Tr}\left(\partial_\alpha H_k\widetilde{\mathcal{U}}^\varepsilon_{\beta,k}(t)\,\gamma_k(0)\,\widetilde{\mathcal{U}}^\varepsilon_{\beta,k}(t)^*\right) - \mathrm{Tr}\left(\partial_\alpha H_k\gamma_k(0)\right) + \varepsilon t\mathrm{Tr}\left(\partial_\alpha H_k\partial_\beta\gamma_k(0)\right)\\ &- i\varepsilon\,\mathrm{Tr}\big(\partial_\alpha H_k(e^{-itL_k}-1)L_k^+\partial_\beta\gamma_k(0)\big).\end{aligned}$$

We now expand the first term in the right-hand side of this equation. We set $\mu := 1 + \min\sigma(H)$,

$$H(s) := H_{k-se_\beta} + \mu, \quad A = \partial_\alpha H_k, \quad I_0 = [0, \frac{1}{2}(\lambda_{N_k,k} + \lambda_{N_k+1,k}) + \mu], \quad P(s) = \mathbb{1}_{I_0}(H(s)).$$

It holds

$$H(s) = h_0 + sh_1 + \frac{s^2|e_\beta|^2}{2}$$

with $h_0 = H_k + \mu$ and $h_1 = J_{\beta,k} = -\partial_\beta H_k$. The operators h_0, h_1 and A are self-adjoint on $L^2_{\rm per}$ and we have $h_0 \ge 1$ and $h_1 h_0^{-1/2}$ and $Ah_0^{-1/2}$ bounded. Besides, $P(s) = \gamma_{k-se_\beta}(0)$, so that $\dot P(0) = -\partial_\beta\gamma_k(0)$. Let $(U^\varepsilon(t,t'))_{t,t'\in\mathbb{R}}$ be the propagator associated with the family $(H(\varepsilon t))_{t\in\mathbb{R}}$ and $U^\varepsilon(t) := U^\varepsilon(t,0)$. We have $U^\varepsilon(t,t') = e^{-i\mu(t-t')}\mathcal{U}^\varepsilon_k(t,t')$ and $U^\varepsilon(t) = e^{-i\mu t}\mathcal{U}^\varepsilon_k(t)$. With these notations, we have

$$\rho^\varepsilon_k(t) = \mathrm{Tr}\left(AU^\varepsilon(t)\,P(0)U^\varepsilon(t)^*\right) - \mathrm{Tr}\left(AP(0)\right) - \varepsilon t\mathrm{Tr}\left(A\dot P(0)\right) + i\varepsilon\,\mathrm{Tr}\Big(A(e^{-itL_0}-1)L_0^+\dot P(0)\Big),$$

where $L_0 = L_{h_0,I_0}$ and $L_0^+ = L^+_{h_0,I_0}$, and we focus on expanding the operator $U^\varepsilon(t)\,P(0)U^\varepsilon(t)^*$ close to $t = 0$.

Lemma 5.8. *We have*

$$U^\varepsilon(t)\,P(0)U^\varepsilon(t)^* = P(0) + \varepsilon\left(t\dot P(0) - i\left(e^{-itL_0}-1\right)\left(L_0^+\dot P(0)\right)\right) + \Pi^\varepsilon_2(t) \tag{79}$$

with $\rho^\varepsilon_k(t) = \mathrm{Tr}\left(A\Pi^\varepsilon_2(t)\right)$. Moreover, we have the bound (78)

$$|\rho^\varepsilon_k(t)| \le C\varepsilon^2 t^3(1+t^3).$$

Lemma 5.8 closes the proof of Proposition 5.7. $\square$

Proof of Lemma 5.8. We deduce from the Dyson expansion that

$$U^\varepsilon(t) = U^0(t) + V^\varepsilon(t) + W^\varepsilon(t),$$

where $U^0(t) = e^{-ith_0}$ and

$$V^\varepsilon(t) = -i\varepsilon \int_0^t U^0(t-t')t'h_1U^0(t')\,dt',$$

$$W^\varepsilon(t) = \varepsilon^2 \left(-i\frac{t^3}{6}U^0(t) + \int_0^t \left(\int_0^{t'} U^\varepsilon(t,t')t'(h_1+\varepsilon t'/2)U^0(t'-t'')t''(h_1+\varepsilon t''/2)U^0(t'')\,dt'' \right) dt' \right).$$

This induces $U^\varepsilon(t)\,P(0)U^\varepsilon(t)^* = P(0) + \Pi_1^\varepsilon(t) + \Pi_2^\varepsilon(t)$ where

$$\Pi_1^\varepsilon(t) = V^\varepsilon(t)P(0)U^0(t)^* + \text{h.c.} = -i\varepsilon \int_0^t t'U^0(t-t')[h_1, P(0)]U^0(t-t')^*\,dt',$$

$$\Pi_2^\varepsilon(t) = V^\varepsilon(t)P(0)V^\varepsilon(t)^* + \big(W^\varepsilon(t)P(0)(U^0(t)+V^\varepsilon(t))^* + \text{h.c.}\big) + W^\varepsilon(t)P(0)W^\varepsilon(t)^*.$$

We first analyze $\Pi_1^\varepsilon(t)$ by computing

$$\begin{aligned} U^0(t-t')[h_1, P(0)]U^0(t-t')^* &= -e^{-i(t-t')L_0}L_0\dot{P}(0) \\ &= i\frac{d}{dt'}e^{-i(t-t')L_0}\dot{P}(0) \\ &= \frac{d^2}{dt'^2}e^{-i(t-t')L_0}L_0^+\dot{P}(0), \end{aligned}$$

where we have used $\dot{P}(0) = L_0^+[P_0, h_1]$ and $\dot{P}(0) = L_0^+L_0\dot{P}(0)$. Using integration by parts, we obtain

$$\Pi_1^\varepsilon(t) = \varepsilon\left(t\dot{P}(0) - i\left(e^{-itL_0}-1\right)\left(L_0^+\dot{P}(0)\right)\right)$$

and (79) follows.

We now work on the bound (78). For that purpose, we introduce the following quantities, which are independent of k, ε and t:

$$\begin{aligned} \nu_0 &= \max_{|e|\le|e_\alpha|,|e_\beta|} \|(J\cdot e)(H+\mu)^{-1/2}\|_{\mathcal{L}(L^2(\mathbb{R}^d;\mathbb{C}))}, \\ \nu_1 &= \max_{|e|\le|e_\alpha|,|e_\beta|} \|(H+\mu)^{1/2}(J\cdot e)(H+\mu)^{-1}\|_{\mathcal{L}(L^2(\mathbb{R}^d;\mathbb{C}))}, \\ \nu_2 &= \max_{|e|\le|e_\alpha|,|e_\beta|} \|(H+\mu)(J\cdot e)(H+\mu)^{-2}\|_{\mathcal{L}(L^2(\mathbb{R}^d;\mathbb{C}))}, \\ \lambda &= \max_{k\in\mathbb{R}^d,|k-k'|\le|e_\beta|} \|(H_k+\mu)^{1/2}(H_{k'}+\mu)^{-1/2}\|_{\mathcal{L}(L^2_{\text{per}})}. \end{aligned}$$

Note that the assumptions $\mathcal{A} \in (L^4_{\text{per}})^d$, $\nabla\cdot\mathcal{A} = 0$, and $V \in L^2_{\text{per}}$ are sufficient to ensure that the quantities ν_0, ν_1 and λ are finite. Besides, since $\|h_0h_1h_0^{-2}\| \le \|(H+\mu)J_\beta(H+\mu)^{-2}\|$ and

$$(H+\mu)J_\beta(H+\mu)^{-2} = J_\beta(H+\mu)^{-1} - 2i\sum_{\alpha=1}^d(\partial_\alpha\mathcal{A}_\beta - \partial_\beta\mathcal{A}_\alpha)J_\alpha(H+\mu)^{-2} - (\Delta\mathcal{A}_\beta)(H+\mu)^{-2} + i\partial_\beta V(H+\mu)^{-2},$$

we deduce from the assumptions $\mathcal{A} \in (H^2_{\text{per}})^d$ and $V \in H^1_{\text{per}}$ that $\|(H+\mu)J_\beta(H+\mu)^{-2}\| < \infty$, hence that $\nu_2 < \infty$.

We now aim at controlling $\rho_k(t)$ thanks to ν_0, ν_1, ν_2 and λ. Using the relations $P(0) = P(0)^2$ and $P(0) = h_0^{-m}h_0^mP(0)$ with

$$\|h_0^mP(0)\| \le (\mu_{\text{F}}+\mu)^m, \quad \|h_0^{-1}\| \le \|h_0^{-1/2}\| \le 1 \quad \text{and } \operatorname{Rank}(P(0)) = N_k \le \overline{N} := \max_{k'} N_{k'},$$

we deduce

$$\begin{aligned} |\rho_k^\varepsilon(t)| \le \overline{N}\Big(&(\mu_{\text{F}}+\mu)^2\|AV^\varepsilon(t)h_0^{-1}\|\,\|V^\varepsilon(t)h_0^{-1}\| + 2(\mu_{\text{F}}+\mu)^3\|AW^\varepsilon(t)h_0^{-2}\|\,(\|h_0^{-1}\| + \|V^\varepsilon(t)h_0^{-1}\|) \\ &+ (\mu_{\text{F}}+\mu)^3\|AW^\varepsilon(t)h_0^{-2}\|\|W^\varepsilon(t)h_0^{-1}\|\Big) \\ \le \overline{N}\nu_0\Big(&(\mu_{\text{F}}+\mu)^2\|h_0^{1/2}V^\varepsilon(t)h_0^{-1}\|^2 + (\mu_{\text{F}}+\mu)^3\|h_0^{1/2}W^\varepsilon(t)h_0^{-2}\|(2+2\|V^\varepsilon(t)h_0^{-1}\| \\ &+ \|W^\varepsilon(t)h_0^{-1}\|)\Big). \end{aligned}$$

Next, we get

$$\|V^\varepsilon(t)h_0^{-1}\| \le \frac{\varepsilon t^2}{2}\|h_1 h_0^{-1}\| \le \frac{\varepsilon t^2}{2}\nu_0, \quad \|h_0^{1/2}V^\varepsilon(t)h_0^{-1}\| \le \frac{\varepsilon t^2}{2}\nu_1,$$
$$\|W^\varepsilon(t)h_0^{-1}\| \le \varepsilon^2 t^3\left(\frac{1}{6}+\nu_0\nu_1\frac{t}{8}+(\varepsilon t)t\left(\frac{\nu_0}{30}+\frac{\nu_1}{20}\right)+(\varepsilon t)^2 t\frac{1}{72}\right),$$
$$\|h_0^{1/2}W^\varepsilon(t)h_0^{-2}\| \le \varepsilon^2 t^3\lambda e^{\eta\varepsilon t/2}\left(\frac{1}{6}+\nu_1\nu_2\frac{t}{8}+(\varepsilon t)t\left(\frac{\nu_1}{30}+\frac{\nu_2}{20}\right)+(\varepsilon t)^2 t\frac{1}{72}\right).$$

It follows that there exists a constant C depending only on V, $\mathcal{A}$ and μ_{F}, such that

$$|\rho_k^\varepsilon(t)| \le C\varepsilon^2 t^3\left(t+e^{\eta\varepsilon t/2}\left(1+t(1+(\varepsilon t)^2)+(\varepsilon t)t^2(1+(\varepsilon t)^3)+(\varepsilon t)^4t^3(1+(\varepsilon t)^2)\right)\right),$$

which leads to (78) when $\varepsilon t \le 1$. $\square$

6 Insulators

In this section and the following ones, we use the notation $O(f(\varepsilon,t,t',\delta))$ to denote a term that is bounded in absolute value by $Cf(\varepsilon,t,t',\delta)$, where C is a constant that can depend on the system under consideration (through $\mathcal{A}$, V, μ_{F}, e_α and e_β), but not on the parameters ε,t,t',δ. We will use the notation γ_k^0 for $\gamma_k(0)$.

We now prove Theorem 2.7. For insulators, $N_k = N_{\mathrm{ins}}$ for all k, and $\lambda_{N_k+1,k}-\lambda_{N_k,k}$, hence g_k, is uniformly bounded away from zero and $s_k=+\infty$. We use the notation L_k^+ for $L_{N_{\mathrm{ins}},k}^+$. We apply Corollary 5.5 and obtain by integrating over the Brillouin zone

$$j_{\alpha,\beta}^\varepsilon(t) = -(2\pi)^{-d}\int_{\mathcal{B}}\partial_\alpha\left(\mathrm{Tr}\Big(H_{k-\varepsilon e_\beta t}\gamma^0_{k-\varepsilon e_\beta t}\Big)\right)dk - i\varepsilon(2\pi)^{-d}\int_{\mathcal{B}}\mathrm{Tr}\Big(\partial_\alpha H_{k-\varepsilon e_\beta t}L^+_{k-e_\beta t}\partial_\beta\gamma^0_{k-\varepsilon e_\beta t}\Big)dk$$
$$+ i\varepsilon(2\pi)^{-d}\int_{\mathcal{B}}\mathrm{Tr}\Big(\partial_\alpha H_{k-\varepsilon e_\beta t}\,\widetilde{\mathcal{U}}^\varepsilon_{\beta,k}(t)\,(L_k^+\partial_\beta\gamma_k^0)\widetilde{\mathcal{U}}^\varepsilon_{\beta,k}(t)^*\Big)dk + O\left(\varepsilon^2 te^{\eta\varepsilon t}\right).$$

As mentioned in Remark 5.6, these three terms are adiabatic, static and oscillatory respectively.

- The first term of the right-hand side vanishes for all t, as the integral of the derivative of the smooth periodic function $k\mapsto \mathrm{Tr}\big(H_k\gamma_k^0\big)$ on a unit cell.
- The second term is dealt with using the relation

  $$L_k^+((\partial_\alpha H_k)^{\mathrm{OD}}) = [\gamma_k^0\ ,\ \partial_\alpha\gamma_k^0],$$

  where $(\partial_\alpha H_k)^{\mathrm{OD}} = \gamma_k^0(\partial_\alpha H_k)(1-\gamma_k^0)+(1-\gamma_k^0)(\partial_\alpha H_k)\gamma_k^0$. By periodicity, we have

  $$\int_{\mathcal{B}}\mathrm{Tr}\left(\partial_\alpha H_{k-\varepsilon e_\beta t}L^+_{k-\varepsilon e_\beta t}\partial_\beta\gamma^0_{k-\varepsilon e_\beta t}\right)dk = \int_{\mathcal{B}}\mathrm{Tr}\left(\partial_\alpha H_k L_k^+\partial_\beta\gamma_k^0\right)dk,$$

  and we observe that

  $$\begin{aligned}\mathrm{Tr}\left(\partial_\alpha H_k L_k^+\partial_\beta\gamma_k^0\right) &= \mathrm{Tr}\left((\partial_\alpha H_k)^{\mathrm{OD}}L_k^+\partial_\beta\gamma_k^0\right)\\ &= \mathrm{Tr}\left(L_k^+((\partial_\alpha H_k)^{\mathrm{OD}})\partial_\beta\gamma_k^0\right) = \mathrm{Tr}\left([\gamma_k^0,\partial_\alpha\gamma_k^0]\partial_\beta\gamma_k^0\right),\end{aligned} \tag{80}$$

  so that

  $$\int_{\mathcal{B}}\mathrm{Tr}\left(\partial_\alpha H_{k-\varepsilon e_\beta t}L^+_{k-\varepsilon e_\beta t}\partial_\beta\gamma^0_{k-\varepsilon e_\beta t}\right)dk = \int_{\mathcal{B}}\mathrm{Tr}\left(\gamma_k^0[\partial_\alpha\gamma_k^0,\partial_\beta\gamma_k^0]\right)dk.$$

- We now focus on the time-average of the oscillating term

  $$\omega^\varepsilon(t) := \frac{1}{t}\int_0^t dt'\int_{\mathcal{B}}\mathrm{Tr}\Big(\partial_\alpha H_{k-\varepsilon e_\beta t'}\,\widetilde{\mathcal{U}}^\varepsilon_{\beta,k}(t')\,(iL_k^+\partial_\beta\gamma_k^0)\widetilde{\mathcal{U}}^\varepsilon_{\beta,k}(t')^*\Big)dk.$$

  In order to bound this term, we apply Lemma 5.4 to $A = iL_k^+\partial_\beta\gamma_k^0$, which is a self-adjoint off-diagonal operator for the decomposition $L^2_{\mathrm{per}} = \mathrm{Ran}(\gamma_k^0)\oplus\mathrm{Ker}(\gamma_k^0)$. We thus get

  $$\widetilde{\mathcal{U}}^\varepsilon_{\beta,k}(t)\left(iL_k^+\partial_\beta\gamma_k^0\right)\widetilde{\mathcal{U}}^\varepsilon_{\beta,k}(t)^* = \frac{d}{dt}\left(iL^+_{k-\varepsilon e_\beta t}\Big(\widetilde{\mathcal{U}}^\varepsilon_{\beta,k}(t)(iL_k^+\partial_\beta\gamma_k^0)\widetilde{\mathcal{U}}^\varepsilon_{\beta,k}(t)^*\Big)\right)+\widetilde{R}_k^\varepsilon(t),$$

where

$$\widetilde{R}_k^\varepsilon(t) = 2\widetilde{\mathcal{U}}_{\beta,k}^\varepsilon(t) r_k^\varepsilon(t)(iL_k^+\partial_\beta\gamma_k^0) r_k^\varepsilon(t)\widetilde{\mathcal{U}}_{\beta,k}^\varepsilon(t)^* - \left(\widetilde{\mathcal{U}}_{\beta,k}^\varepsilon(t)(1-2\gamma_k^0)(iL_k^+\partial_\beta\gamma_k^0) r_k^\varepsilon(t)\widetilde{\mathcal{U}}_{\beta,k}^\varepsilon(t)^* + \text{h.c.}\right)$$
$$- \varepsilon i\partial_\beta L^+_{k-\varepsilon te_\beta}\widetilde{\mathcal{U}}_{\beta,k}^\varepsilon(t)(iL_k^+\partial_\beta\gamma_k^0)\widetilde{\mathcal{U}}_{\beta,k}^\varepsilon(t))^*$$

and

$$r_k^\varepsilon(t) = i\varepsilon\widetilde{\mathcal{U}}_{\beta,k}^\varepsilon(t)^*\left(L^+_{k-\varepsilon te_\beta}\partial_\beta\gamma^0_{k-\varepsilon te_\beta}\right)\widetilde{\mathcal{U}}_{\beta,k}^\varepsilon(t) - i\varepsilon L_k^+\partial_\beta\gamma_k^0 + \widetilde{\mathcal{U}}_{\beta,k}^\varepsilon(t)^* R_k^\varepsilon(t)\widetilde{\mathcal{U}}_{\beta,k}^\varepsilon(t),$$

where $R_k^\varepsilon(t)$ is defined in (76). Therefore,

$$\begin{aligned}
&\mathrm{Tr}\Big(\partial_\alpha H_{k-\varepsilon e_\beta t}\widetilde{\mathcal{U}}_{\beta,k}^\varepsilon(t)\ (iL_k^+\partial_\beta\gamma_k^0)\widetilde{\mathcal{U}}_{\beta,k}^\varepsilon(t)^*\Big)\\
&\quad= \mathrm{Tr}\left(\partial_\alpha H_{k-\varepsilon e_\beta t}\frac{d}{dt}\left(\widetilde{\mathcal{U}}_{\beta,k}^\varepsilon(t)\ (iL_k^+\partial_\beta\gamma_k^0)\widetilde{\mathcal{U}}_{\beta,k}^\varepsilon(t)^*\right)\right) + \mathrm{Tr}\left(\partial_\alpha H_{k-\varepsilon e_\beta t}\widetilde{R}_k^\varepsilon(t)\right)\\
&\quad= \frac{d}{dt}\,\mathrm{Tr}\left(\partial_\alpha H_{k-\varepsilon e_\beta t}\left(\widetilde{\mathcal{U}}_{\beta,k}^\varepsilon(t)\ (iL_k^+\partial_\beta\gamma_k^0)\widetilde{\mathcal{U}}_{\beta,k}^\varepsilon(t)^*\right)\right) + \mathrm{Tr}\left(\partial_\alpha H_{k-\varepsilon e_\beta t}\widetilde{R}_k^\varepsilon(t)\right)
\end{aligned}$$

since

$$\begin{aligned}
\mathrm{Tr}\left(\frac{d}{dt}(\partial_\alpha H_{k-\varepsilon e_\beta t})\,\widetilde{\mathcal{U}}_{\beta,k}^\varepsilon(t)\ (iL_k^+\partial_\beta\gamma_k^0)\widetilde{\mathcal{U}}_{\beta,k}^\varepsilon(t)^*\right) &= -\varepsilon\,\mathrm{Tr}\left(\partial_{k_\alpha k_\beta}H_{k-\varepsilon e_\beta t}\widetilde{\mathcal{U}}_{\beta,k}^\varepsilon(t)\ (iL_k^+\partial_\beta\gamma_k^0)\widetilde{\mathcal{U}}_{\beta,k}^\varepsilon(t)^*\right)\\
&= -\varepsilon e_\alpha\cdot e_\beta\,\mathrm{Tr}\left(\widetilde{\mathcal{U}}_{\beta,k}^\varepsilon(t)\ (iL_k^+\partial_\beta\gamma_k^0)\widetilde{\mathcal{U}}_{\beta,k}^\varepsilon(t)^*\right)\\
&= -\varepsilon e_\alpha\cdot e_\beta\,\mathrm{Tr}\left(iL_k^+\partial_\beta\gamma_k^0\right) = 0,
\end{aligned}$$

where we have used the fact that $\partial_{k_\alpha k_\beta}H_k = -e_\alpha\cdot e_\beta$ and the off-diagonal character of $iL_k^+\partial_\beta\gamma_k^0$. Hence, using the bounds from Proposition 5.1, we obtain

$$\begin{aligned}
\omega^\varepsilon(t) &= \frac{1}{t}\int_{\mathcal{B}}\mathrm{Tr}\left(\partial_\alpha H_{k-\varepsilon e_\beta t}\left(\widetilde{\mathcal{U}}_{\beta,k}^\varepsilon(t)\ (iL_k^+\partial_\beta\gamma_k^0)\widetilde{\mathcal{U}}_{\beta,k}^\varepsilon(t)^*\right)\right)dk + \frac{1}{t}\int_0^t dt'\int_{\mathcal{B}}\mathrm{Tr}\left(\partial_\alpha H_{k-\varepsilon e_\beta t'}\widetilde{R}_k^\varepsilon(t')\right)dk\\
&= O\left(\left(\frac{1}{t}+\varepsilon\right)e^{\eta\varepsilon t}\right).
\end{aligned}$$

The result follows.

7 Metals

We prove the two assertions of Theorem 2.8 in sequence.

7.1 Linear response

We prove the first assertion of Theorem 2.8: We first note that, for $\varepsilon > 0$ small enough and $t \le \frac{1}{\varepsilon}\varepsilon^\theta$, the function $k \mapsto \lambda_{N_k+1,k-\varepsilon e_\beta t} - \lambda_{N_k,k-\varepsilon e_\beta t}$ is bounded away from zero, and therefore so is $g_k(\varepsilon t)$. We can therefore apply Corollary 5.5 on each B_N to obtain

$$\begin{aligned}
j^\varepsilon_{\alpha,\beta}(t) = (2\pi)^{-d}\sum_{N\in\mathbb{N}}\Bigg(&-\int_{B_N}\mathrm{Tr}\big(\partial_\alpha H_{k-\varepsilon e_\beta t}P_{N,k-\varepsilon e_\beta t}\big)dk\\
&-i\varepsilon\int_{B_N}\mathrm{Tr}\Big(\partial_\alpha H_{k-\varepsilon e_\beta t}L^+_{k-\varepsilon e_\beta t}\partial_\beta P_{N,k-\varepsilon e_\beta t}\Big)dk\\
&+i\varepsilon\int_{B_N}\mathrm{Tr}\Big(\partial_\alpha H_{k-\varepsilon e_\beta t}\widetilde{\mathcal{U}}_{\beta,k}^\varepsilon(t)\ L_k^+\partial_\beta P_{N,k}\widetilde{\mathcal{U}}_{\beta,k}^\varepsilon(t)^*\Big)dk\Bigg)\\
&+O\left(\varepsilon^2 te^{\eta\varepsilon t}\right)
\end{aligned} \tag{81}$$

and so

$$j^\varepsilon_{\alpha,\beta}(t) = -(2\pi)^{-d}\sum_{N\in\mathbb{N}}\int_{B_N}\mathrm{Tr}\big(\partial_\alpha H_{k-\varepsilon e_\beta t}P_{N,k-\varepsilon e_\beta t}\big)dk + O(\varepsilon) \tag{82}$$

when $t \leq \frac{1}{\varepsilon}\varepsilon^\theta$. In contrast to the case of insulators however, the adiabatic term

$$-(2\pi)^{-d} \sum_{N\in\mathbb{N}} \int_{\mathcal{B}_N} \partial_\alpha \operatorname{Tr}\big(H_{k-\varepsilon e_\beta t} P_{N,k-\varepsilon e_\beta t}\big) dk = \varepsilon t (2\pi)^{-d} \sum_{N\in\mathbb{N}} \int_{\mathcal{B}_N} \partial_\alpha \partial_\beta \left(\operatorname{Tr}(H_k P_{N,k})\right) dk + O(\varepsilon^2 t^2)$$

has a non-zero first-order contribution (the zeroth-order term vanishes by Proposition 2.1). The proportionality factor is computed by the Stokes formula as

$$\begin{aligned}\sum_{N\in\mathbb{N}^*} \int_{\mathcal{B}_N} \partial_\alpha\partial_\beta \operatorname{Tr}\big(H_k \gamma_k^0\big) dk &= \sum_{N\in\mathbb{N}^*} \int_{\mathcal{B}_N} \partial_\alpha\partial_\beta \sum_{n=1}^{N} \lambda_{n,k} = \sum_{N\in\mathbb{N}^*} \left(\int_{\mathcal{S}_N} - \int_{\mathcal{S}_{N-1}}\right) \partial_\alpha \sum_{n=1}^{N} \lambda_{n,k} (ds\cdot e_\beta) \\ &= \sum_{N\in\mathbb{N}^*} \int_{\mathcal{S}_N} \partial_\alpha \lambda_{N,k} (ds \cdot e_\beta) = (2\pi)^d D_{\alpha,\beta} \end{aligned} \tag{83}$$

and the result follows.

7.2 Bloch oscillations

Under the assumptions of the second assertion, N_k is either N_{met} or $N_{\text{met}}-1$, and in both cases

$$\lambda_{N_k+1,k-\varepsilon e_\beta t} - \lambda_{N_k,k-\varepsilon e_\beta t}$$

is bounded away from zero uniformly in k,t. We can therefore apply Corollary 5.5 and obtain

$$j^\varepsilon_{\alpha,\beta}(t) = -(2\pi)^{-d} \sum_{N\in\mathbb{N}} \int_{\mathcal{B}_N} \left(\partial_\alpha \operatorname{Tr}\big(H_{k-\varepsilon e_\beta t} P_{N_k,k-\varepsilon e_\beta t}\big)\right) dk + O((\varepsilon+\varepsilon^2 t)\mathrm{e}^{\eta\varepsilon t}).$$

From the decomposition

$$P_{N_k,k-\varepsilon e_\beta t} = P_{N_{\text{met}}-1,k-\varepsilon e_\beta t} + \mathbb{1}(\lambda_{N_{\text{met}},k} \leq \mu_{\mathrm{F}}) |u_{N_{\text{met}},k-\varepsilon e_\beta t}\rangle\langle u_{N_{\text{met}},k-\varepsilon e_\beta t}|$$

and since $k \mapsto P_{N_{\text{met}}-1,k-\varepsilon e_\beta t}$ is smooth and $\mathcal{R}^*$-periodic, we have

$$\begin{aligned} j^\varepsilon_{\alpha,\beta}(t) &= -(2\pi)^{-d} \int_{\mathcal{B}} \mathbb{1}(\lambda_{N_{\text{met}},k} \leq \mu_{\mathrm{F}}) \langle u_{N_{\text{met}},k-\varepsilon e_\beta t} | \partial_\alpha H_{k-\varepsilon e_\beta t} | u_{N_{\text{met}},k-\varepsilon e_\beta t}\rangle dk + O((\varepsilon+\varepsilon^2 t)\mathrm{e}^{\eta\varepsilon t}) \\ &= -(2\pi)^{-d} \int_{\mathcal{B}} \mathbb{1}(\lambda_{N_{\text{met}},k} \leq \mu_{\mathrm{F}}) \partial_\alpha \lambda_{N_{\text{met}},k-\varepsilon e_\beta t} dk + O((\varepsilon+\varepsilon^2 t)\mathrm{e}^{\eta\varepsilon t}), \end{aligned}$$

which concludes the proof.

8 Semi-metals

We prove here Theorem 2.10. We decompose the integral defining $j^\varepsilon_{\alpha,\beta}(t)$ into several parts depending whether one integrates far from the Dirac points or not.

We introduce a small parameter $\delta > 0$ controlling the size of the neighborhood of the Dirac points, which is independent of t, ε. We decompose $\mathcal{B}$ as the disjoint union

$$\mathcal{B} = \mathcal{B}^\delta_{\text{out}} \cup (\cup_{i\in\mathcal{I}} \mathcal{B}^\delta_i)$$

with

$$\mathcal{B}^\delta_i = B(k_i, \delta),$$

where $\delta > 0$ is small enough so that

$$\mathcal{B}^\delta_{\text{out}} \subset \{k \in \mathcal{B},\ \lambda_{N_{\text{sm}},k} \leq \mu_F - c\delta\}$$

for some constant $c > 0$. Note that this decomposition is time-reversal symmetric in the sense that

$$-\mathcal{B}^\delta_{\text{out}} = \mathcal{B}^\delta_{\text{out}} \ \text{ and } \ -(\cup_{i\in\mathcal{I}} \mathcal{B}^\delta_i) = (\cup_{i\in\mathcal{I}} \mathcal{B}^\delta_i).$$

We work in the regime $\varepsilon t \ll \delta \ll 1$, $\varepsilon \ll \delta \ll 1$.

In the following analysis, we first treat the regions $\mathcal{B}^\delta_{\text{out}}$, where we will use adiabatic theory with a non-zero gap larger than a constant times δ. In the sets $\mathcal{B}^\delta_i$, where the gap closes, we study the structure of the Taylor expansion of the Hamiltonian H_k close to the Dirac points and construct two-band reduced Hamiltonians $H^R_{i,k}$. Then, we use the linear response Proposition 5.7, reducing successively from the Hamiltonian H to the reduced Hamiltonian $H^R_{i,k}$, and finally to the Dirac Hamiltonian

$$H^D_k = \begin{pmatrix} 0 & k_1 - ik_2 \\ k_1 + ik_2 & 0 \end{pmatrix}$$

for which we can explicitly compute the current. Adding the contributions, we will obtain

$$\sigma_{\alpha,\beta} := \lim_{t\to\infty} \lim_{\varepsilon\to 0} \frac{1}{\varepsilon t} \int_0^t j^\varepsilon_{\alpha,\beta}(t')dt' = \frac{|\mathcal{I}|}{16} e_\alpha \cdot e_\beta + O(\delta)$$

Finally, we will pass to the limit $\delta \to 0$.

8.1 Far from the Dirac points

We set

$$j^{\varepsilon,\mathrm{out}}_{\alpha,\beta}(t') := -\frac{1}{4\pi^2} \int_{\mathcal{B}^\delta_{\mathrm{out}}} \mathrm{Tr}\left(\partial_\alpha H_k \widetilde{\mathcal{U}}^\varepsilon_{\beta,k}(t')\, \gamma^0_k\, \widetilde{\mathcal{U}}^\varepsilon_{\beta,k}(t')^*\right) dk.$$

Let $k \in \mathcal{B}^\delta_{\mathrm{out}}$. In the regime we consider, $\gamma^0_{k-\varepsilon e_\beta t} = P_{N_{\mathrm{sm}},k-\varepsilon e_\beta t}$ is gapped with a gap larger than a constant times δ. Applying the analysis of the previous sections, we obtain that

$$\begin{aligned} -\mathrm{Tr}&\left(\partial_\alpha H_k \widetilde{\mathcal{U}}^\varepsilon_{\beta,k}(t)\, \gamma^0_k\, \widetilde{\mathcal{U}}^\varepsilon_{\beta,k}(t)^*\right) \\ &= -\partial_\alpha\left(\mathrm{Tr}\Big(H_{k-\varepsilon e_\beta t}\gamma^0_{k-\varepsilon e_\beta t}\Big)\right) - i\varepsilon\, \mathrm{Tr}\Big(\partial_\alpha H_{k-\varepsilon e_\beta t} L^+_{k-\varepsilon e_\beta t}\partial_\beta \gamma^0_{k-\varepsilon e_\beta t}\Big) \\ &\quad + i\varepsilon\, \mathrm{Tr}\Big(\partial_\alpha H_{k-\varepsilon e_\beta t}\widetilde{\mathcal{U}}^\varepsilon_{\beta,k}(t)\left(L^+_k \partial_\beta \gamma^0_k\right)\widetilde{\mathcal{U}}^\varepsilon_{\beta,k}(t)^*\Big) + O\left(\varepsilon^2 t \delta^{-6}\right). \end{aligned}$$

We treat each term separately.

- For the first (adiabatic) term, we have

$$\begin{aligned} -\partial_\alpha\, \mathrm{Tr}\Big(H_{k-\varepsilon e_\beta t}\gamma^0_{k-\varepsilon e_\beta t}\Big) &= -\partial_\alpha\, \mathrm{Tr}\big(H_k \gamma^0_k\big) + \varepsilon t \partial_\alpha \partial_\beta\, \mathrm{Tr}\big(H_k\gamma^0_k\big) \\ &\quad + O\left(\varepsilon^2 t^2 \delta^{-4}\right). \end{aligned}$$

  By time-reversal symmetry, the first term vanishes when integrated on $\mathcal{B}^\delta_{\mathrm{out}}$. Using Stokes formula for the second term as in the metallic case, we get

$$\int_{\mathcal{B}^\delta_{\mathrm{out}}} -\partial_\alpha\left(\mathrm{Tr}\Big(H_{k-\varepsilon e_\beta t}\gamma^0_{k-\varepsilon e_\beta t}\Big)\right) dk = \varepsilon t \sum_{n\le N_{\mathrm{sm}}} \int_{\partial\mathcal{B}^\delta_{\mathrm{in}}} \partial_\alpha \lambda_{n,k}(ds\cdot e_\beta) + O\left(\varepsilon^2 t^2\delta^{-4}\right) \tag{84}$$

- For the second (static) term we similarly expand in ε

$$\begin{aligned} -i\varepsilon \int_{\mathcal{B}^\delta_{\mathrm{out}}} \mathrm{Tr}\Big(\partial_\alpha H_{k-\varepsilon e_\beta t} L^+_{k-\varepsilon e_\beta t}\partial_\beta\gamma^0_{k-\varepsilon e_\beta t}\Big) dk &= -i\varepsilon \int_{\mathcal{B}^\delta_{\mathrm{out}}} \mathrm{Tr}\left(\gamma^0_k[\partial_\alpha\gamma^0_k, \partial_\beta\gamma^0_k]\right) dk + O(\varepsilon^2 t\delta^{-6}) \\ &= O(\varepsilon^2 t \delta^{-6}), \end{aligned}$$

  where we used the fact that the function $k \mapsto \mathrm{Tr}\left(\gamma^0_k[\partial_\alpha\gamma^0_k, \partial_\beta\gamma^0_k]\right)$ is odd.

- For the third (oscillatory) term, we use the same arguments as in the insulating case, and obtain

$$\frac{1}{t}\int_0^t dt' \int_{\mathcal{B}^\delta_{\mathrm{out}}} i\varepsilon\, \mathrm{Tr}\Big(\partial_\alpha H_{k-\varepsilon e_\beta t'}\widetilde{\mathcal{U}}^\varepsilon_{\beta,k}(t')\left(L^+_k\partial_\beta\gamma^0_k\right)\widetilde{\mathcal{U}}^\varepsilon_{\beta,k}(t')^*\Big) dk = O\left(\varepsilon\delta^{-6}\left(\frac{1}{t} + \varepsilon\right)\right).$$

We are left with

$$\begin{aligned} \frac{1}{t}\int_0^t j^{\varepsilon,\mathrm{out}}_{\alpha,\beta}(t')\,dt' &= \frac{\varepsilon}{4\pi^2 t}\int_0^t t'dt' \sum_{n\le N_{\mathrm{sm}}} \int_{\partial\mathcal{B}^\delta_{\mathrm{in}}} \partial_\alpha\lambda_{n,k}(ds\cdot e_\beta) + O\left(\frac{\varepsilon}{\delta^6}\left(\frac{1}{t} + \varepsilon(1+t^2)\right)\right) \\ &= \frac{\varepsilon t}{2\pi^2} \sum_{n\le N_{\mathrm{sm}}} \int_{\partial\mathcal{B}^\delta_{\mathrm{in}}} \partial_\alpha\lambda_{n,k}(ds\cdot e_\beta) + O\left(\frac{\varepsilon}{\delta^6}\left(\frac{1}{t} + \varepsilon(1+t^2)\right)\right). \end{aligned} \tag{85}$$

8.2 Close to Dirac points: reduction to the 2-band case

We set

$$j^{\varepsilon,\mathrm{in}}_{\alpha,\beta}(t) := -\frac{1}{4\pi^2}\sum_{i\in\mathcal{I}}\int_{\mathcal{B}^\delta_{\mathrm{in}}} \mathrm{Tr}\left(\partial_\alpha H_k \widetilde{\mathcal{U}}^\varepsilon_{\beta,k}(t)\,\gamma^0_k \widetilde{\mathcal{U}}^\varepsilon_{\beta,k}(t)^*\right) dk. \tag{86}$$

Using the linear response Proposition 5.7, we have for almost all $k \in \mathcal{B}^\delta_{\mathrm{in}}$ and all $\varepsilon, t \geq 0$,

$$\begin{aligned}-\mathrm{Tr}\left(\partial_\alpha H_{k-\varepsilon e_\beta t}\widetilde{\mathcal{U}}^\varepsilon_{\beta,k}(t)\,\gamma^0_k \widetilde{\mathcal{U}}^\varepsilon_{\beta,k}(t)^*\right) = &-\partial_\alpha \mathrm{Tr}\left(H_k\gamma^0_k\right) + \varepsilon t \partial_\alpha\partial_\beta\left(\mathrm{Tr}\big(H_k\gamma^0_k\big)\right)\\ &- i\varepsilon\,\mathrm{Tr}\big(\partial_\alpha H_k (e^{-itL_k}-1)L_k^+\partial_\beta\gamma^0_k\big) + O(\varepsilon^2 t^3(1+t^3)).\end{aligned}$$

Using (72), the equality $\mathrm{Tr}\left(H_k\gamma^0_k\right) = \sum_{n=1}^{N_{\mathrm{sm}}}\lambda_{n,k}$ and Assumption 2.6, it is easily seen that the left-hand side, as well as the first and fourth terms of the right-hand side of that equation, are bounded uniformly in k and therefore integrable on $\mathcal{B}^\delta_i$. Besides, for $k\in\mathcal{B}^\delta_{\mathrm{in}}$, the second term is bounded by a constant multiple of $(1/|k-k_i|)$ as $k\to k_i$, and is therefore integrable. It follows that the third term is also integrable on $\mathcal{B}^\delta_i$.

We treat the three leading terms of the right-hand side in sequence.

- The first term vanishes when integrated on the time-reversal symmetric set $\cup_{i\in\mathcal{I}}\mathcal{B}^\delta_i$.
- For the second, arguing as in the metallic case, we get

  $$\int_{\mathcal{B}^\delta_i}\varepsilon t\partial_{\alpha\beta}\left(\mathrm{Tr}\big(H_k\gamma^0_k\big)\right)dk = -\varepsilon t\sum_{n\leq N_{\mathrm{sm}}}\int_{\partial\mathcal{B}^\delta_i}\partial_\alpha\lambda_{n,k}(ds\cdot e_\beta),$$

  so that the corresponding term in (86) cancels the contribution (85) from $\mathcal{B}^\delta_{\mathrm{out}}$.
- For the third term, we use

  $$\begin{aligned}&\mathrm{Tr}\big(\partial_\alpha H_k(e^{-itL_k}-1)L_k^+\partial_\beta\gamma^0_k\big) = \mathrm{Tr}\big(\partial_\alpha H_k(e^{-itL_k}-1)(L_k^+)^2[\gamma^0_k,\partial_\beta H_k]\big)\\ &= \sum_{n\leq N_{\mathrm{sm}}}\sum_{m>N_{\mathrm{sm}}}(e^{-it(\lambda_{n,k}-\lambda_{m,k})}-1)\frac{\langle u_{n,k},\partial_\beta H_k u_{m,k}\rangle\langle u_{m,k},\partial_\alpha H_k u_{n,k}\rangle}{(\lambda_{m,k}-\lambda_{n,k})^2} - \text{c.c.}\end{aligned}$$

  with the sum converging from the asymptotics (16).
  When $n \neq N_{\mathrm{sm}}$ or $m\neq N_{\mathrm{sm}}+1$, the denominators in that equation are bounded from below independently of δ. The constant term vanishes when integrated over the time-reversal symmetric set $\cup_{i\in\mathcal{I}}\mathcal{B}^\delta_i$, and the oscillatory term can be treated using the formula

  $$\frac{1}{t}\int_0^t e^{-i\omega t'}dt' = \frac{e^{-i\omega t}-1}{-i\omega t}$$

  with $\omega = \lambda_{n,k}-\lambda_{m,k}$ bounded away from zero independently of δ.

Putting all the results of the previous two sections together, we get that

$$\begin{aligned}\frac{1}{t}\int_0^t j^\varepsilon_{\alpha,\beta}(t')dt' &= \frac{1}{t}\int_0^t j^{\varepsilon,\mathrm{out}}_{\alpha,\beta}(t')dt' + \frac{1}{t}\int_0^t j^{\varepsilon,\mathrm{in}}_{\alpha,\beta}(t')dt'\\ &= -\frac{i\varepsilon}{4\pi^2 t}\sum_{i\in\mathcal{I}}\int_0^t dt'\int_{\mathcal{B}^\delta_i}(e^{-it'(\lambda_{N_{\mathrm{sm}},k}-\lambda_{N_{\mathrm{sm}}+1,k})}-1)\\ &\qquad\times\frac{\langle u_{N_{\mathrm{sm}},k},\partial_\beta H_k u_{N_{\mathrm{sm}}+1,k}\rangle\langle u_{N_{\mathrm{sm}}+1,k},\partial_\alpha H_k u_{N_{\mathrm{sm}},k}\rangle}{(\lambda_{N_{\mathrm{sm}}+1,k}-\lambda_{N_{\mathrm{sm}},k})^2}dk - \text{c.c.}\\ &\quad + O\left(\varepsilon^2\delta^{-6}(1+t^2)+\varepsilon\delta^{-6}t^{-1}+\varepsilon^2t^3(1+t^3)\right).\end{aligned}$$

At this stage of the proof, only two modes are involved in the formula giving the current, namely the two modes that cross at the Fermi level. Everything happens as for a two-band model that we now study. We write for short

$$\frac{1}{t}\int_0^t\frac{j^\varepsilon_{\alpha,\beta}(t')}{\varepsilon}dt' = -\frac{i}{4\pi^2 t}\sum_{i\in\mathcal{I}}\int_0^t I^{R,i}_{\alpha,\beta}(t')\,dt' + O\left(\varepsilon\delta^{-6}(1+t^2)+\delta^{-6}t^{-1}+\varepsilon t^3(1+t^3)\right),$$

with

$$I^{R,i}_{\alpha,\beta}(\delta,t) = \int_{\mathcal{B}^\delta_i}(e^{-it(\lambda_{N_{\mathrm{sm}},k}-\lambda_{N_{\mathrm{sm}}+1,k})}-1)\frac{\langle u_{N_{\mathrm{sm}},k},\partial_\beta H_k u_{N_{\mathrm{sm}}+1,k}\rangle\langle u_{N_{\mathrm{sm}}+1,k},\partial_\alpha H_k u_{N_{\mathrm{sm}},k}\rangle}{(\lambda_{N_{\mathrm{sm}}+1,k}-\lambda_{N_{\mathrm{sm}},k})^2}dk - \text{c.c.}.$$

8.3 Close to the Dirac points: the local model

We now are interested in the computation of $I^{R,i}_{\alpha,\beta}(t)$. In the following, we drop the index i and assume without loss of generality that $k_i = 0$.

Hypothesis (33) implies that, for k small enough, the Bloch Hamiltonian H_k has exactly two eigenvalues (counting multiplicities) close to $\mu_{\rm F}$. Consider an arbitrary orthonormal basis (v_0, w_0) of $\mathrm{Ran}(P_{N_{\rm sm}+1,0}-P_{N_{\rm sm}-1,0})$. For all k small enough, we can construct an orthonormal basis (v_k, w_k) of $\mathrm{Ran}(P_{N_{\rm sm}+1,k}-P_{N_{\rm sm}-1,k})$ by Löwdin orthonormalization of $((P_{N_{\rm sm}+1,k}-P_{N_{\rm sm}-1,k})v_0, (P_{N_{\rm sm}+1,k}-P_{N_{\rm sm}-1,k})w_0)$, and set

$$H^R_k = [v_k|w_k]^* H_k [v_k|w_k] = \begin{pmatrix} \langle v_k, H_k v_k\rangle & \langle v_k, H_k w_k\rangle \\ \langle w_k, H_k v_k\rangle & \langle w_k, H_k w_k\rangle \end{pmatrix}.$$

It follows that the reduced Hamiltonian

$$H_k\Big|_{\mathrm{Ran}(P_{N_{\rm sm}+1,k}-P_{N_{\rm sm}-1},k)}$$

is equivalent through a unitary transform that depends analytically on k to the reduced 2×2 Hamiltonian

$$H^R_k = \sum_{p=0}^{3} b^p(k)\sigma_p, \tag{87}$$

where

$$\sigma_0 = \mathrm{Id}_{\mathbb{C}^2},\quad \sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix},\quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix},\quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

are the Pauli matrices, and $(b^p)_{p=0,1,2,3}$ are real-valued analytic functions of k in a neighborhood of 0.

The matrix H^R_k has eigenvalues

$$\lambda_\pm(k) = b^0(k) \pm \sqrt{\sum_{p=1}^{3} b^p(k)^2}.$$

It follows that

$$b^0(k) = \mu_F + O(|k|^2),\quad b^p(k) = v_F\langle q^p, k\rangle + O(|k|^2),\quad p = 1,2,3,$$

where the $(q^p)_{p=1,2,3}$ are the rows of a 3×2 matrix Q with orthogonal columns, so that

$$H^R_k = \mu_F + v_F(Qk)\cdot\sigma + O(|k|^2). \tag{88}$$

Let $R \in \mathrm{SO}(3)$ be a rotation matrix that maps $\mathrm{Ran}(Q)$ to $\mathrm{Span}(e^0_1, e^0_2)$, where (e^0_1, e^0_2, e^0_3) is the canonical basis of $\mathbb{R}^3$. Let U be one of its associated 2×2 unitary matrices through the two-to-one $\mathrm{SU}(2)\to\mathrm{SO}(3)$ mapping, so that [7]

$$R_{pq} = \frac{1}{2}\,\mathrm{Tr}(\sigma_p U \sigma_q U^*).$$

It follows that

$$\begin{aligned} \mathrm{Tr}\big(\sigma_3 U H^R_k U^*\big) &= v_F \sum_{q=1}^{3} (Qk)_q\,\mathrm{Tr}(\sigma_3 U\sigma_q U^*) + O(|k|^2) \\ &= 2v_F \sum_{q=1}^{3} \langle e^0_3, RQk\rangle + O(|k|^2) \\ &= O(|k|^2). \end{aligned}$$

Up to a unitary transform, we can therefore assume Q to be a 2×2 matrix in (88).

8.4 The two-band case: reduction to the Dirac Hamiltonian

Reduction to H_k^R For $k \neq 0$, let $\lambda^R_{\pm,k}$ be the larger and smaller eigenvalues of H_k^R respectively, and $u^R_{\pm,k}$ associated orthonormal eigenvectors in $\mathbb{C}^2$. We have $\lambda^R_{-,k} = \lambda_{N_{\rm sm},k}$, $\lambda^R_{+,k} = \lambda_{N_{\rm sm}+1,k}$, and

$$[v_k|w_k]u^R_{+,k} = e^{i\theta_+(k)}u_{N_{\rm sm}+1,k}, \qquad [v_k|w_k]u^R_{-,k} = e^{i\theta_-(k)}u_{N_{\rm sm},k}$$

for some phases $\theta_\pm(k) \in \mathbb{R}$. We have

$$\begin{aligned}\partial_\alpha H_k^R &= [v_k|w_k]^*\partial_\alpha H_k[v_k|w_k] + \partial_\alpha[v_k|w_k]^*[v_k|w_k]H_k^R + H_k^R[v_k|w_k]^*\partial_\alpha[v_k|w_k] \\ &= [v_k|w_k]^*\partial_\alpha H_k[v_k|w_k] + O(|k|)\end{aligned}$$

where we have used for the first line that H_k commutes with $P_{N_{\rm sm}+1,k} - P_{N_{\rm sm},k} = [v_k|w_k][v_k|w_k]^*$, and for the second that $H_k^R = \mu_F \mathrm{Id}_2 + O(|k|)$ and $\partial_\alpha\Big([v_k|w_k]^*[v_k|w_k]\Big) = \partial_\alpha \mathrm{Id}_2 = 0$. We therefore obtain

$$\begin{aligned}\langle u^R_{+,k}, \partial_\alpha H_k^R u^R_{-,k}\rangle &= e^{-i(\theta_+(k)-\theta_-(k))}\langle u_{N_{\rm sm}+1,k}, \partial_\alpha H_k u_{N_{\rm sm},k}\rangle + O(|k|) \\ \langle u^R_{-,k}, \partial_\beta H_k^R u^R_{+,k}\rangle &= e^{+i(\theta_+(k)-\theta_-(k))}\langle u_{N_{\rm sm},k}, \partial_\beta H_k u_{N_{\rm sm}+1,k}\rangle + O(|k|).\end{aligned}$$

Since $(\lambda^R_{-,k} - \lambda^R_{+,k})$ is bounded from below by a constant multiple of $|k|$, it follows that

$$I^R_{\alpha,\beta}(\delta,t) = \int_{B(0,\delta)} (e^{-it(\lambda^R_{-,k}-\lambda^R_{+,k})} - 1)\frac{\langle u^R_{-,k}, \partial_\beta H_k^R u^R_{+,k}\rangle\langle u^R_{+,k}, \partial_\alpha H_k^R u^R_{-,k}\rangle}{(\lambda^R_{+,k} - \lambda^R_{-,k})^2}dk - \text{c.c.} + O(\delta). \quad (89)$$

Reduction to H_k^D By standard results of perturbation theory [21] applied to $H_k^R = \mu_F + v_F(Qk)\cdot\sigma + O(|k|^2)$ with gap greater than a constant multiple of $|k|$,

$$\lambda^R_{\pm,k} = \lambda^Q_{\pm,k} + O(|k|^2) \ \text{ and } \ u^R_{\pm,k} = u^Q_{\pm,k} + O(|k|)$$

where the superscript Q refers to eigenvalues and appropriately chosen orthonormal eigenvectors of the Hamiltonian

$$H_k^Q = v_F(Qk)\cdot\sigma.$$

It follows that

$$I^R_{\alpha,\beta}(\delta,t) = I^Q_{\alpha,\beta}(\delta,t) + O(\delta),$$

where $I^R_{\alpha,\beta}(\delta,t)$ is defined similarly to (89) as

$$I^Q_{\alpha,\beta}(\delta,t) = \int_{B(0,\delta)} (e^{-it(\lambda^Q_{-,k}-\lambda^Q_{+,k})} - 1)\frac{\langle u^Q_{-,k}, \partial_\beta H_k^Q u^Q_{+,k}\rangle\langle u^Q_{+,k}, \partial_\alpha H_k^Q u^Q_{-,k}\rangle}{(\lambda^Q_{+,k} - \lambda^Q_{-,k})^2}dk - \text{c.c.}.$$

We perform the change of variable $k' = Qk$ (recall that Q is orthogonal) and obtain

$$I^Q_{\alpha,\beta}(\delta,t) = e_\beta^T\, I^D(\delta,t)e_\alpha,$$

where the coefficients $I^D_{ij}(\delta,t)$ of the 2×2 matrix $I^D(\delta,t)$ are given by

$$I^D_{ij}(\delta,t) = \int_{B(0,\delta)} (e^{-it(\lambda^D_{-,k}-\lambda^D_{+,k})} - 1)\frac{\langle u^D_{-,k}, \partial_{k_j} H_k^D u^D_{+,k}\rangle\langle u^D_{+,k}, \partial_{k_i} H_k^D u^D_{-,k}\rangle}{(\lambda^D_{+,k} - \lambda^D_{-,k})^2}dk - \text{c.c.}$$

and the superscript D refers to the Dirac Hamiltonian

$$H_k^D = v_F k\cdot\sigma.$$

The Dirac Hamiltonian H_k^D We finish by computing $I^D(\delta,t)$ explicitly. Let $k = r(\cos\theta,\sin\theta)$. We have

$$\lambda^D_{\pm,k} = \pm v_F r, \ \ u^D_{+,k} = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\ e^{i\theta}\end{pmatrix} \ \text{ and } \ u^D_{-,k} = \frac{1}{\sqrt{2}}\begin{pmatrix}-e^{-i\theta}\\ 1\end{pmatrix}.$$

By an explicit calculation, we obtain

$$\int_0^{2\pi} (e^{-it(\lambda^D_{-,k}-\lambda^D_{+,k})}-1)\frac{\langle u^D_{-,k}, \partial_{k_i} H^D_k u^D_{+,k}\rangle\langle u^D_{+,k}, \partial_{k_j} H^D_k u^D_{-,k}\rangle}{(\lambda^D_{+,k}-\lambda^D_{-,k})^2}\, d\theta - \text{c.c.} = i\pi\frac{1}{2r^2}\sin(2v_F rt)\delta_{ij}.$$

It follows that

$$\begin{aligned}\frac{1}{t}\int_0^t I^D_{ij}(\delta,t')\,dt' &= \frac{i\pi}{2}\delta_{ij}\frac{1}{t}\int_0^t\int_0^\delta \frac{\sin(2v_F rt')}{r}\,dr\,dt' = \frac{i\pi}{4t}\delta_{ij}\int_0^\delta \frac{1-\cos(2v_F rt)}{v_F r^2}\,dr\\ &= \frac{i\pi}{4}\delta_{ij}\int_0^{\delta v_F t}\frac{1-\cos(2r')}{(r')^2}\,dr' = \frac{i\pi^2}{4}\delta_{ij} + O\left((\delta t)^{-1}\right).\end{aligned}$$

We finally get by summing all the estimates

$$\frac{1}{t}\int_0^t \frac{j^\varepsilon_{\alpha,\beta}(t')}{\varepsilon}\,dt' = \frac{|\mathcal{I}|}{16}e_\alpha\cdot e_\beta + O\left(\delta + \varepsilon t^3(1+t^3) + \frac{1}{\delta^6}\left(\frac{1}{t}+\varepsilon(1+t)^2\right)\right),$$

hence the result.

A Proofs of two technical lemmata

A.1 Proof of Lemma 4.1

Proof. We replicate the proof of the Faris-Lavine Theorem given in [32], replacing the Laplacian by $\frac{1}{2}(-i\nabla+\mathcal{A})^2$. It consists in verifying the following two hypotheses of [32, Theorem X.37]. Let $A = \frac{1}{2}(-i\nabla+\mathcal{A})^2 + W + V$ and $N = A + 2c|x|^2 + b$, where $b\in\mathbb{R}$ will be specified below:

$$\textit{there exists } h\textit{, such that for any } \phi\in\mathcal{C},\quad \|A\phi\|\le h\|N\phi\|; \tag{90}$$

$$\textit{for some } \ell\textit{, for any } \phi\in\mathcal{C},\quad |(A\phi,N\phi)-(N\phi,A\phi)|\le \ell\|N^{\frac{1}{2}}\phi\|^2. \tag{91}$$

By hypothesis *3* in Lemma 4.1 and the conditions on W, it is possible to choose b so that $N\ge 1$. As quadratic forms on $\mathcal{C}$,

$$N^2 = (A+b)^2 + 4c\sum_{j=1}^d x_j(A+b+c|x|^2)x_j - 2cd.$$

Hypotheses *1* and *3* guarantee that $A+b+c|x|^2$ is bounded below. Hence, increasing the value of b if necessary to make this operator positive, we have

$$\|(A+b)\phi\|^2_{L^2}\le \|N\phi\|^2_{L^2} + 4cd\|\phi\|^2_{L^2},$$

which proves (90).

For (91), we observe that

$$\pm i[A,N] = \pm 2c(x\cdot(-i\nabla+\mathcal{A}) + (-i\nabla+\mathcal{A})\cdot x) \le 2c\left((-i\nabla+\mathcal{A})^2+|x|^2\right)\le \ell N,$$

where we have used

$$(-i\nabla+\mathcal{A})^2 + |x|^2 \pm (x\cdot(-i\nabla+\mathcal{A}) + (-i\nabla+\mathcal{A})\cdot x) = (-i\nabla+\mathcal{A}\pm x)^2\ge 0$$

and

$$N = \left(\frac{a}{2}(-i\nabla+\mathcal{A})^2+V\right) + (W+c|x|^2) + \frac{1-a}{2}(-i\nabla+\mathcal{A})^2 + c|x|^2 + b \ge e((-i\nabla+\mathcal{A})^2+|x|^2),$$

where $e=\min(c,\frac{1-a}{2})>0$ and where b is chosen so that

$$b - f + \min\sigma\left(\frac{a}{2}(-i\nabla+\mathcal{A})^2+V\right)\ge 0.$$

This proves (91). Hence A is essentially self-adjoint on $\mathcal{C}$. □

A.2 Proof of Lemma 4.2

Proof. By the Kato-Rellich theorem, for any $0 \leq t \leq T$, $H(t)$ is self-adjoint on L^2_{per} with domain H^2_{per}, and bounded below. We will show that there exists $\mu > 0$ so that the graph norm of $(H(t) + \mu)$ for any $0 \leq t \leq T$ is equivalent to the H^2_{per}-norm. This will prove Lemma 4.2 by Proposition 2.1 in [36] (see also Theorem X.70 in [32]).

We have for any $\mu > 0$, $0 \leq t \leq T$ and $\phi \in H^2_{\mathrm{per}}$,

$$\|(H(t)+\mu)\phi\|_{L^2_{\mathrm{per}}} \leq (1+a)\|H_0\phi\|_{L^2_{\mathrm{per}}} + (b+\mu)\|\phi\|_{L^2_{\mathrm{per}}} \leq (1+a+b+\mu)\|\phi\|_{H^2_{\mathrm{per}}},$$

and so the graph norm is controlled by the H^2_{per}-norm.

For the other inequality, we relate the resolvent of $H(t)$ to that of H_0 by a bounded operator, with bounded inverse. Notice that, for any $\mu > 0$, since H_0 is positive,

$$\forall\, 0 \leq t \leq T, \quad (H(t)+\mu) = (1 + H_1(t)(H_0+\mu)^{-1})(H_0+\mu).$$

Furthermore,

$$\forall\, 0 \leq t \leq T, \quad \|H_1(t)(H_0+\mu)^{-1}\| \leq a\|H_0(H_0+\mu)^{-1}\| + b\|(H_0+\mu)^{-1}\| \leq a + \frac{b}{\mu}.$$

and so, for $\mu > \frac{b}{1-a}$, the operator $1 + H_1(t)(H_0+\mu)^{-1}$ is bounded and invertible with bounded inverse in L^2_{per}. Therefore $(H(t)+\mu)^{-1}$ is bounded from L^2_{per} to H^2_{per}, which means there exists $C > 0$ such that, for any $\phi \in H^2_{\mathrm{per}}$ and $0 \leq t \leq T$,

$$\|\phi\|_{H^2_{\mathrm{per}}} = \|(H(t)+\mu)^{-1}(H(t)+\mu)\phi\|_{H^2_{\mathrm{per}}} \leq C\|(H(t)+\mu)\phi\|_{L^2_{\mathrm{per}}},$$

which concludes the proof. □

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